

3/18/05

10/666811f.

Structure Search

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\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 20:16:44 ON 18 MAR 2005

=> fil reg

COST IN U.S. DOLLARS

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 20:16:53 ON 18 MAR 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAR 2005 HIGHEST RN 845858-62-0

DICTIONARY FILE UPDATES: 17 MAR 2005 HIGHEST RN 845858-62-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

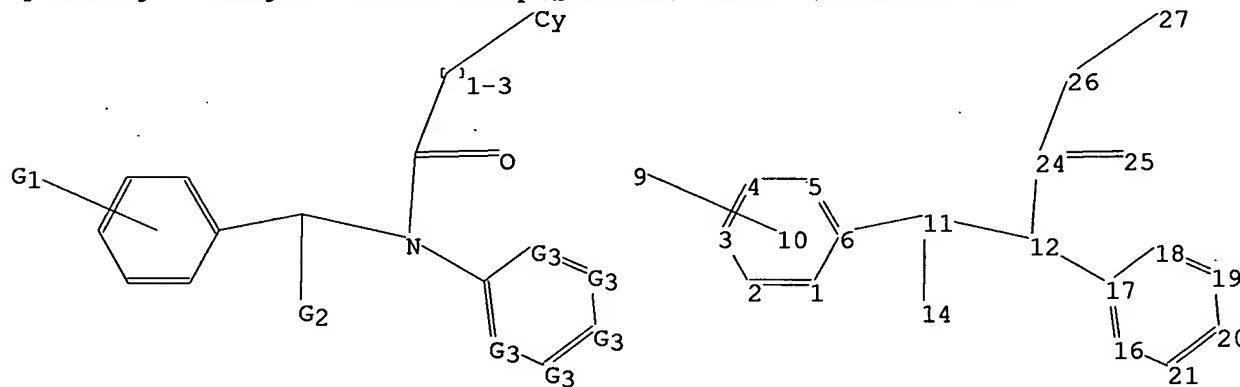
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10666811\10666811f.str



chain nodes :

9 11 12 14 24 25 26 27

ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21

chain bonds :

6-11 11-12 11-14 12-17 12-24 24-25 24-26 26-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

6-11 11-12 11-14 12-17 12-24 16-17 16-21 17-18 18-19 19-20 20-21 24-25  
24-26 26-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:H,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CN,X,Ak

G2: Ak, H

G3: C, N

Hydrogen count :

11: >= minimum 1

Match level :

1: Atom 2: Atom 3: Atom 4: Atom 5: Atom 6: Atom 9: CLASS 10: CLASS 11: CLASS

12: CLASS 14: CLASS 16: Atom 17: Atom 18: Atom 19: Atom 20: Atom 21: Atom 24: CLASS

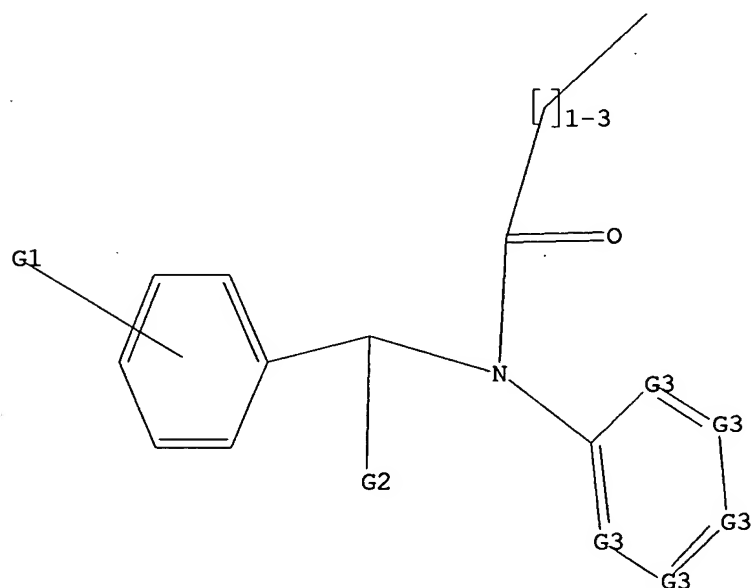
25: CLASS 26: CLASS 27: Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 H,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CN,X,Ak

G2 Ak, H

G3 C, N

Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 20:17:45 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2061 TO ITERATE

48.5% PROCESSED 1000 ITERATIONS 32 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 38497 TO 43943  
PROJECTED ANSWERS: 832 TO 1806

L2 32 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 20:18:04 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 41486 TO ITERATE

100.0% PROCESSED 41486 ITERATIONS 1241 ANSWERS  
SEARCH TIME: 00.00.02

L3 1241 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.76	161.97

FILE 'CAPLUS' ENTERED AT 20:18:12 ON 18 MAR 2005  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 18 Mar 2005 VOL 142 ISS 13  
FILE LAST UPDATED: 17 Mar 2005 (20050317/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3

L4 174 L3

=> d L4 ibib abs hitstr 160-174

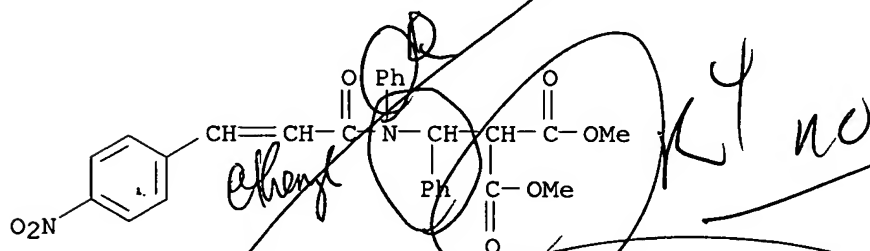
L4 ANSWER 160 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1966:75311 CAPLUS  
DOCUMENT NUMBER: 64:75311

(2,4-dinitrophenylhydrazones m. 152°) and isobutyric acid. VI under the same conditions gave a  $\gamma$ -diketone, C<sub>9</sub>H<sub>16</sub>O<sub>2</sub>, b<sub>25</sub> 72°; bis(2,4-dinitrophenylhydrazone) m. 155°. IVa was similarly converted into 2,5-dimethyl-3-isopropyl-2-(2-methyl-3-butenyl)-5-hydroxytetrahydrofuran (VII), b<sub>0.7</sub> 98-103°. A mixture of 140 g. 2,3,3,5-tetramethyl-2-isobutenyl-2,3-dihydrofuran (VIII), 48 ml. 95% AcOH, and 41.5 g. fused NaOAc was heated at 60° for 3 hrs. to give 2,3,3,5-tetramethyl-2-isobutenyl-5-hydroxytetrahydrofuran (IX), b<sub>1</sub> 70-5°, n<sub>18D</sub> 1.4692. Hydrogenation of IV in 0.5N KOH-alc. in the presence of Raney Ni at 80°/90 kg. for 20 hrs. gave 6-methyl-7-propyl-6,9-decanediol (X), b<sub>1.5</sub> 140°. Under similar conditions, VII and IX gave, resp., 2,5-dimethyl-6-isopropyl-5,8-nonanediol (XI), b<sub>1</sub> 126-30°, and 2,4,5,5-tetramethyl-2-octene-4,7-diol (XII), m. 74-5° (petr. ether), b<sub>0.8</sub> 126, n<sub>20D</sub> 1.4650, d<sub>20</sub> 0.989. IX under the same conditions, but in the absence of alkali, was hydrogenated to 2,3,3,5-tetramethyl-2-isobutenyltetrahydrofuran (XIII). Hydrogenation of IV in 0.1N KOH-alc. with PtO<sub>2</sub> catalyst at 20°/90 kg. for 7 hrs. gave 2,5-dimethyl-3-propyl-2-pentyltetrahydrofuran. Under similar conditions, IX gave 2,3,3,5-tetramethyl-2-isobutyltetrahydrofuran (XIV), m. 93°. VII under similar conditions but in the absence of alkali gave 2,5-dimethyl-3-isopropyl-2-isobutyltetrahydrofuran, b<sub>1</sub> 75°. XII (10 g.) in 15 ml. ether hydrogenated at 100°/100 kg. for 6 hrs. in the presence of PtO<sub>2</sub> gave XIV. XII (3 g.) oxidized with CrO<sub>3</sub>-C<sub>5</sub>H<sub>5</sub>N at room temperature overnight gave VIII, b<sub>13</sub> 75°, n<sub>20D</sub> 1.3591. Similar treatment of X, XI, and iso-BuCMe(OH)CMe<sub>2</sub>CH<sub>2</sub>CHMeOH gave, resp., 2,5-dimethyl-3-propyl-2-pentyl-2,3-dihydrofuran (XV), b<sub>1</sub> 78°, 2,5-dimethyl-3-isopropyl-2-isoamyl-2,3-dihydrofuran (XVI), b<sub>7</sub> 82°, and 2,3,3,5-tetramethyl-2-isobutyl-2,3-dihydrofuran (XVII), b<sub>15</sub> 78°, n<sub>19D</sub> 1.4500, d<sub>20</sub> 0.862. XV, XVI, and XVII in the presence of AcOH or ZnO were isomerized to 6-methylene-7-propyl-9-decanone, b<sub>7</sub> 111°, 2-methyl-5-methylene-6-isopropyl-8-nonanone, b<sub>7</sub> 105-110°, and 2,5,5-trimethyl-4-methylene-7-octanone, b<sub>4</sub> 64-6° (semicarbazone m. 150-5°), resp.

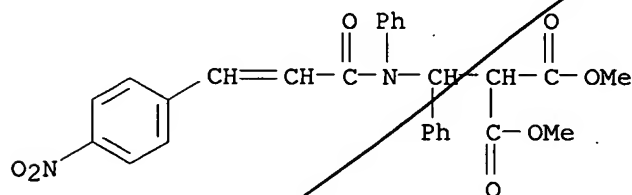
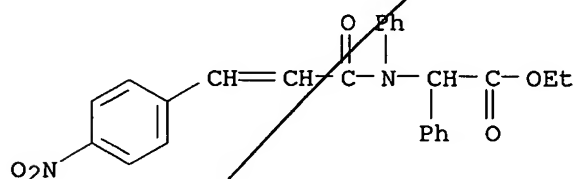
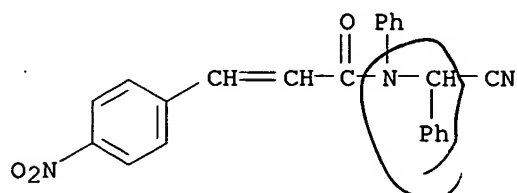
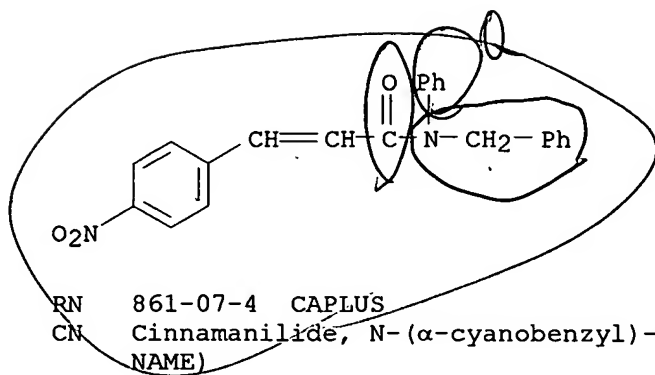
IT 864-29-9, Malonic acid, [ $\alpha$ -(p-nitro-N-phenylcinnamamido)benzyl]-, dimethyl ester (preparation of)

RN 864-29-9 CAPLUS

CN Malonic acid, [ $\alpha$ -(p-nitro-N-phenylcinnamamido)benzyl]-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 166 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1965:74078 CAPLUS  
 DOCUMENT NUMBER: 62:74078  
 ORIGINAL REFERENCE NO.: 62:13108d-h,13109a-b  
 TITLE: Lactams. IV. New synthesis of  $\beta$ -lactams  
 AUTHOR(S): Bose, Ajay K.; Manhas, M. S.; Ramer, R. M.  
 CORPORATE SOURCE: Stevens Inst. Technol., Hoboken, NJ  
 SOURCE: Tetrahedron (1965), 21(3), 449-55  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 62:74078



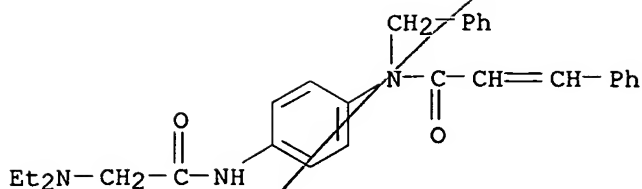
L4 ANSWER 167 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1965:51733 CAPLUS  
DOCUMENT NUMBER: 62:51733  
ORIGINAL REFERENCE NO.: 62:9153a-e  
TITLE: 1,4-Diazines  
PATENT ASSIGNEE(S): CIBA Ltd.  
SOURCE: 25 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO.

DATE



● HCl

L4 ANSWER 173 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:53133 CAPLUS

DOCUMENT NUMBER: 56:53133

ORIGINAL REFERENCE NO.: 56:10029b-e

TITLE: V had antihistaminic and spasmolytic but no anesthetic activity. II

AUTHOR(S): Carelli, Vineenzo; Cardellini, Mario; Liberatore, Felice

CORPORATE SOURCE: Univ. Rome

SOURCE: Annali di Chimica (Rome, Italy) (1961), 51, 707-12

CODEN: ANCRAI; ISSN: 0003-4592

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Preparation of p- $\text{O}_2\text{NC}_6\text{H}_4\text{NHC}_6\text{H}_4\text{COCH:CHPh}$  (VI) was described. To 6 g.  $\text{PhNHCH}_2\text{Ph}$  in 100 cc.  $\text{C}_6\text{H}_6$  was added 5 g.  $\text{K}_2\text{CO}_3$  and with stirring 5.5 g. II in 50 cc.  $\text{C}_6\text{H}_6$ . Refluxing 8 h., cooling, filtering, washing with 10%  $\text{NaOH}$ , 10%  $\text{HCl}$ , and water, evaporating, and distilling yielded 9.5 g. VI ( $\text{R} = \text{H}$ ), b.p. 195-7°, m. 94-5° (ligroine). Similarly, from 30 g. p- $\text{O}_2\text{NC}_6\text{H}_4\text{NHC}_6\text{H}_4\text{COCH:CHPh}$  and 26 g. II was obtained 45 g. VI ( $\text{R} = \text{NO}_2$ , m. 115-16° (ligroine).  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  (140 g.) in 600 cc. water, 40 cc. concentrated  $\text{HCl}$ , and 15 g. VI ( $\text{R} = \text{NO}_2$ ) was heated on a water bath, stirred, and treated with concentrated  $\text{NH}_3$  to alkalinity. Heating 10 h. with addition at intervals of  $\text{NH}_3$ , leaving 12 h., filtering, extracting the precipitate with

boiling

$\text{EtOH}$ , treating with Norit, and concentrating gave VI ( $\text{R} = \text{NH}_2$ ), m. 178-9° ( $\text{EtOH}$ );  $\text{HCl}$  salt m. 264-6° ( $\text{EtOH}$ ). VI ( $\text{R} = \text{NH}_2$ ) (1 g.) in 50 cc.

xylene treated with 1.6 g.  $\text{Et}_2\text{NCH}_2\text{CH}_2\text{Cl}$ , the mixture refluxed 24 h., 0.5 g.  $\text{K}_2\text{CO}_3$  added, refluxed 12 h., filtered hot, evaporated, taken up with petr. ether, the solution filtered, evaporated, and the residue crystallized from

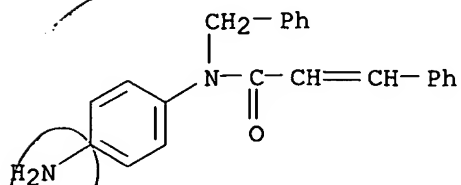
50% aqueous

$\text{EtOH}$  gave VI ( $\text{R} = \text{Et}_2\text{NCH}_2\text{CH}_2\text{NH}$ ), m. 86-8°. Treating slowly 2 g. VI ( $\text{R} = \text{NH}_2$ ) in 25 cc.  $\text{C}_6\text{H}_6$  with 0.7 g.  $\text{ClCH}_2\text{COCl}$  and 0.5 g.  $\text{NaHCO}_3$ , refluxing 5 h., filtering hot, and evapg, gave 1.8 g. VI ( $\text{R} = \text{ClCH}_2\text{CONH}$ ), m. 104-5° ( $\text{EtOH}$ ). Refluxing 10 h. 1.2 g. VI ( $\text{R} = \text{ClCH}_2\text{CONH}$ ) and 0.9 g.  $\text{Et}_2\text{NH}$  in 20 cc.  $\text{C}_6\text{H}_6$ , cooling, filtering, and evaporating gave obtained 1.2 g. VI ( $\text{R} = \text{Et}_2\text{NCH}_2\text{CONH}$ ), m. 134-5° (ligroine), L.D. 50 600 mg./kg. [ $\text{HCl}$  salt m. 189-90° ( $\text{Me}_2\text{CO}$ )], which had anesthetic activity 5 times greater than Novocaine.

IT 100411-13-0, Cinnamanilide, 4'-amino-N-benzyl- 100411-14-1, Cinnamanilide, 4'-amino-N-benzyl-, hydrochloride 100770-78-3, Cinnamanilide, N-benzyl-4'-nitro- 100978-95-8, Cinnamanilide, N-benzyl- 102380-06-3, Cinnamanilide, N-benzyl-4'-[[2-(diethylamino)ethyl]amino]- (preparation of)

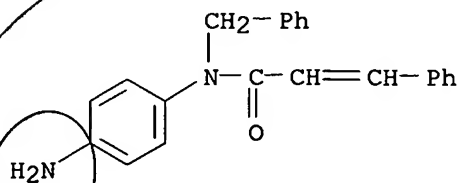
RN 100411-13-0 CAPLUS

CN Cinnamanilide, 4'-amino-N-benzyl- (7CI) (CA INDEX NAME)



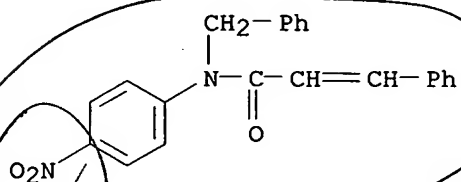
RN 100411-14-1 CAPLUS  
 CN Cinnamanilide, 4'-amino-N-benzyl-, hydrochloride (7CI) (CA INDEX NAME)

Yes



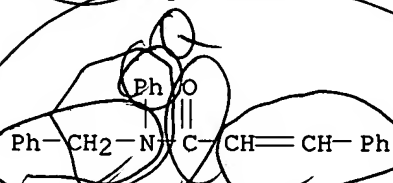
RN 100770-78-3 CAPLUS  
 CN Cinnamanilide, N-benzyl-4'-nitro- (7CI) (CA INDEX NAME)

Yes



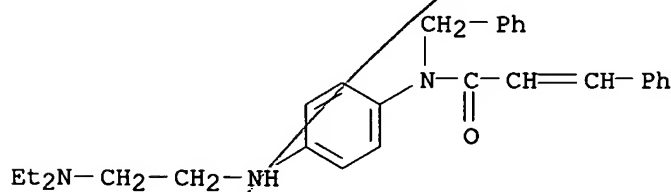
RN 100978-95-8 CAPLUS  
 CN 2-Propenamide, N,3-diphenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Yes



RN 102380-06-3 CAPLUS  
 CN Cinnamanilide, N-benzyl-4'-[[2-(diethylamino)ethyl]amino]- (7CI) (CA INDEX NAME)

Yes 1, 2



L4 ANSWER 174 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1960:11299 CAPLUS

DOCUMENT NUMBER: 54:11299  
ORIGINAL REFERENCE NO.: 54:2270e-i  
TITLE: N-Acylbenzylaminophenols  
PATENT ASSIGNEE(S): J. R. Geigy Akt.-Ges.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 811130		19590402	GB	
DE 1122076			DE	

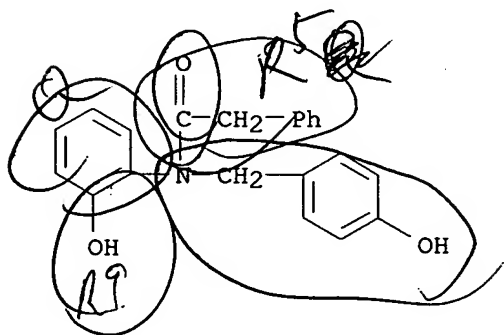
AB The title compds. having antiphlogistic properties are prepared by treating an appropriate acyl halide or other carboxylic acid derivative with N-(p'-hydroxybenzyl)-p-aminophenol (I) in the presence of an acid binding or condensing agent and an inert solvent. I 10 (from reduction of the condensation product of p-aminophenol and p-hydroxybenzaldehyde, m. 155-6°), added to a mixture of Ac2O 4.59, NaOAc 3.85, and glacial AcOH 6.14 parts at 15-25°, stirred 2 hrs., the mixture taken up in H2OEt2O, washed with dilute HCl, extracted with dilute NaOH, and reacidified gave

N-(p-hydroxybenzyl)-N-(p-hydroxyphenyl)acetamide, m. 139-40° (80% EtOH). BzCl and I gave the benzamide of I, m. 189.5-90.5° (H2O-EtOH) and dibutylacetyl chloride with I gave the dibutylacetamide of I, m. 177.5-8.5° (80% EtOH). The following amide derivs. of I can also be prepared (m.p. given): 4-chlorobenzamide, 198-9°; 2-hydroxybenzamide, 183-5°; phenoxyacetamide, 176-7°; cinnamic acid amide, 227-9°; α-phenylpropionamide, 147-80°; α-phenylmercaptobutyramide, 124-5°; caproic acid amide, 147-8°; α-(cyclohepten-1-yl)butyramide, 177-8° α-ethylthiopropionamide, 144-5°; 4-isopropoxybenzamide, 204-6°; isobutyramide, 214-15°; 2-acetyloxybenzamide, 150-5° 2-methylbenzamide, 222-4°; 4-benzyloxybenzamide, 193-5°; stearamide, 120-2°; 3,4,5-trimethoxybenzamide, 231-3° 4-hydroxybenzamide-C6H6, 85-90°; 4-tert-butylbenzamide, 196-8°; 4-butoxybenzamide, 87-8°; acetyloxyacetamide, 70-1°; and 3,4-dimethylbenzamide, 198-200°. N-(p-hydroxybenzyl)-N-(o-hydroxyphenyl)amides include: benzamide, 181-3° dibutylacetamide, 177-8°; phenytacetamide, 181-3°; acetamide, 165-6°; and butyramide, 134-6°. N-(o-hydroxybenzyl)-N-(p-hydroxyphenyl)amides are: benzamide, 180.5-2.5°; acetamide, 142-4°; dibutylacetamide, 181-2.5°; isobutyramide, 172-4°; acetyloxyacetamide, 155-7°.

IT 102479-09-4, Acetanilide, 2'-hydroxy-N-p-hydroxybenzyl-2-phenyl- 112687-84-0, 1-Cycloheptene-1-acetanilide, α-ethyl-4'-hydroxy-N-p-hydroxybenzyl- 112689-41-5, Hydrocinnamanilide, 4'-hydroxy-N-p-hydroxybenzyl- 115020-32-1, Cinnamanilide, 4'-hydroxy-N-p-hydroxybenzyl- (preparation of)

RN 102479-09-4 CAPLUS

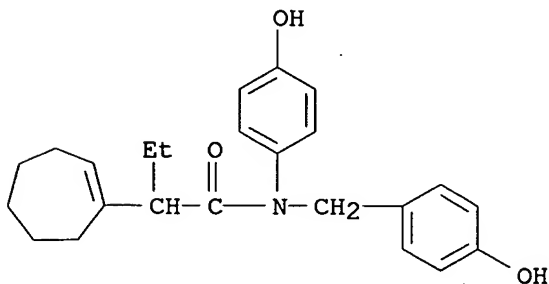
CN Acetanilide, 2'-hydroxy-N-p-hydroxybenzyl-2-phenyl- (6CI) (CA INDEX NAME)



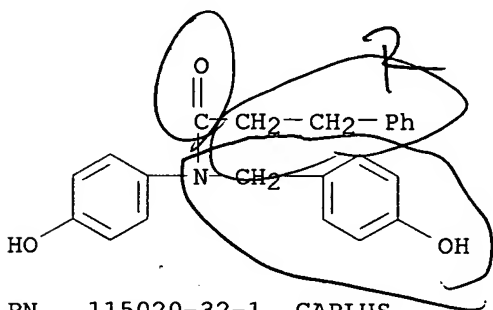
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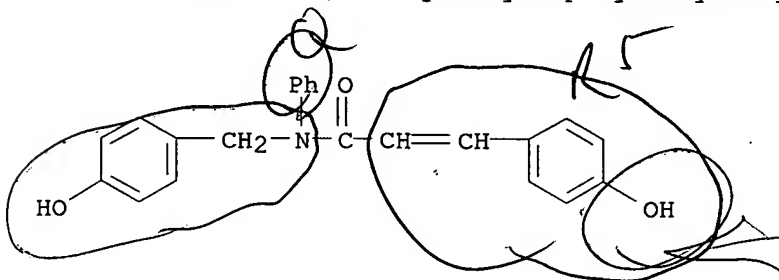
RN 112687-84-0 CAPLUS  
 CN 1-Cycloheptene-1-acetanilide,  $\alpha$ -ethyl-4'-hydroxy-N-p-hydroxybenzyl-  
 (6CI) (CA INDEX NAME)



RN 112689-41-5 CAPLUS  
 CN Hydrocinnamanilide, 4'-hydroxy-N-p-hydroxybenzyl- (6CI) (CA INDEX NAME)



RN 115020-32-1 CAPLUS  
 CN Cinnamanilide, 4'-hydroxy-N-p-hydroxybenzyl- (6CI) (CA INDEX NAME)



yes  
 not 3 but yes 4

=> d cost

COST IN U.S. DOLLARS

CONNECT CHARGES

NETWORK CHARGES

SEARCH CHARGES

DISPLAY CHARGES

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

IN FILE 'CAPLUS' AT 20:20:27 ON 18 MAR 2005

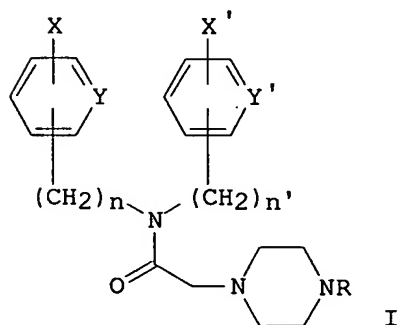
SINCE FILE	TOTAL
ENTRY	SESSION
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0.24	0.42
0.00	160.90
74.10	74.10
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75.90	237.87

SINCE FILE	TOTAL
ENTRY	SESSION
-10.95	-10.95

=> d L4 ibib abs hitstr 100-159

L4 ANSWER 100 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:229087 CAPLUS  
 DOCUMENT NUMBER: 122:31560  
 TITLE: Diaryl piperazineacetamides as antimuscarinic agents  
 INVENTOR(S): Van Hijfte, Luc; Richards, Mary; Hibert, Marcel;  
 Hoflack, Jan; Trumpp-kallmeyer, Susanne; Marciniak,  
 Gilbert  
 PATENT ASSIGNEE(S): Merrell Dow Pharmaceuticals, Inc., USA  
 SOURCE: Eur. Pat. Appl., 55 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 585500	A1	19940309	EP 1992-402435	19920904
R: EP WO 9405648	A1	19940317	WO 1993-US7198	19930729
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 658157	A1	19950621	EP 1993-918532	19930729
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08501096	T2	19960206	JP 1993-507184	19930729
HU 71890	A2	19960228	HU 1995-664	19930729
AU 668413	B2	19960502	AU 1993-47953	19930729
AU 9347953	A1	19940329		
ZA 9306362	A	19940328	ZA 1993-6362	19930830
FI 9501009	A	19950303	FI 1995-1009	19950303
NO 9500842	A	19950303	NO 1995-842	19950303
PRIORITY APPLN. INFO.:			EP 1992-402435	A 19920904
			WO 1993-US7198	W 19930729
OTHER SOURCE(S):	MARPAT 122:31560			
GI				



AB Diaryl piperazineacetamides I (X, X' = H, halo, alkyl, cyanoalkyl, carboxyalkyl, heterocyclylalkyl, etc.; Y, Y' = C, N; n, n' = 0, 1; R = H, alkyl) and their salts useful as antimuscarinic agents for treating a variety of indications such as Parkinson's disease, motion sickness and for the inhibition of gastric acid secretion were prepared. Thus, N,N-diphenyl-4-methyl-1-piperazine dioxalate was prepared by refluxing N,N-diphenylchloroacetamide with N-methylpiperazine in MeCN followed by

treatment with oxalic acid. Appropriate tests to determination the affinity of I to muscarinic receptors are presented.

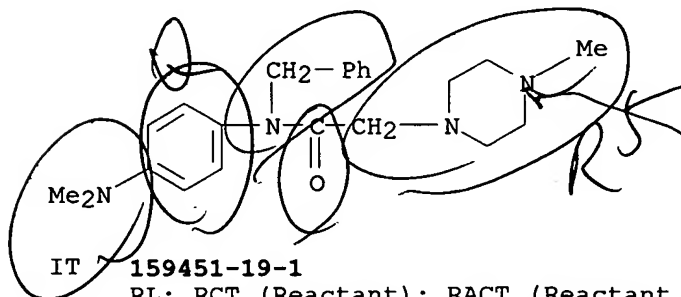
IT 159451-18-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of piperazineacetamides as antimuscarinic agents)

RN 159451-18-0 CAPLUS

CN 1-Piperazineacetamide, N-[4-(dimethylamino)phenyl]-4-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 159451-19-1

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation as antimuscarinic agent)

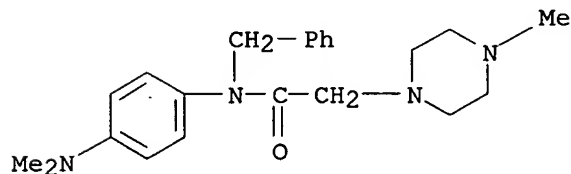
RN 159451-19-1 CAPLUS

CN 1-Piperazineacetamide, N-[4-(dimethylamino)phenyl]-4-methyl-N-(phenylmethyl)-, ethanedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 159451-18-0

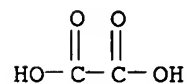
CMF C22 H30 N4 O



CM 2

CRN 144-62-7

CMF C2 H2 O4



L4 ANSWER 101 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:134462 CAPLUS

DOCUMENT NUMBER: 120:134462

TITLE: Heterocyclic phenoxyacetic acid derivative antithrombotic and antihypertensive agents

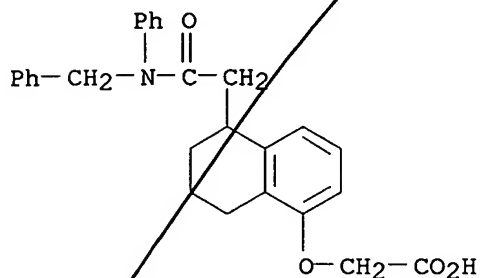
INVENTOR(S): Hamanaka, Nobuyuki; Takahashi, Kanji; Tokumoto, Hidekado

PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan

(preparation of, as PGI2 receptor agonist)

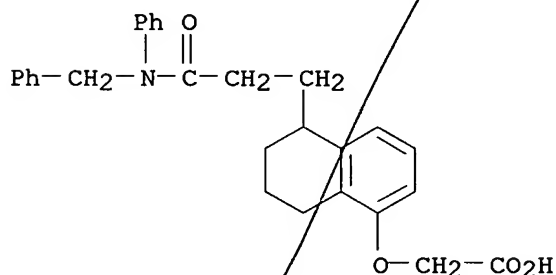
RN 149170-99-0 CAPLUS

CN Acetic acid, [[5,6,7,8-tetrahydro-5-[2-oxo-2-[phenyl(phenylmethyl)amino]ethyl]-1-naphthalenyl]oxy]- (9CI) (CA INDEX NAME)



RN 149171-05-1 CAPLUS

CN Acetic acid, [[5,6,7,8-tetrahydro-5-[3-oxo-3-[phenyl(phenylmethyl)amino]propyl]-1-naphthalenyl]oxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 106 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:233679 CAPLUS

DOCUMENT NUMBER: 118:233679

TITLE: Preparation of herbicidal acetanilides

INVENTOR(S): Goto, Toshio; Hayakawa, Hidenori; Manabe, Itsuko; Yanagi, Akihiko

PATENT ASSIGNEE(S): Nihon Bayer Agrochem K.K., Japan

SOURCE: Eur. Pat. Appl., 26 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

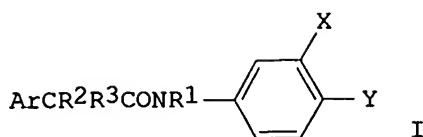
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 521365	A1	19930107	EP 1992-110472	19920622
R: BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
JP 05065258	A2	19930319	JP 1991-268607	19910920
AU 9218455	A1	19930107	AU 1992-18455	19920622
US 5296454	A	19940322	US 1992-905944	19920626
CA 2072780	AA	19930104	CA 1992-2072780	19920630
ZA 9204908	A	19930428	ZA 1992-4908	19920702
BR 9202592	A	19930316	BR 1992-2592	19920703
PRIORITY APPLN. INFO.:			JP 1991-188238	A 19910703
			JP 1991-193647	A 19910709
			JP 1991-268607	A 19910920

OTHER SOURCE(S):  
GI

MARPAT 118:233679



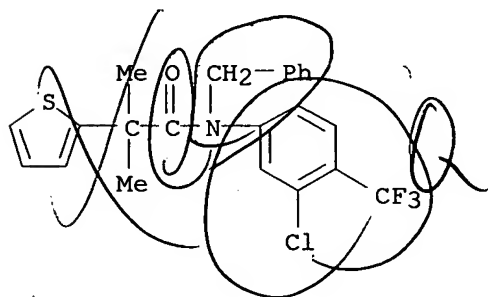
AB Title compds. I (Ar = Ph, furyl, thienyl; R<sup>1</sup> = H, C1-5 alkyl, C3-6 cycloalkyl, C3-6 cycloalkylmethyl, C3-5-alkenyl, C3-5 alkynyl, etc.; R<sup>2</sup>, R<sup>3</sup> = H, C1-3 alkyl; X = halo; Y = Me<sub>2</sub>CH, Me<sub>3</sub>C, C1-2 haloalkyl, -haloalkoxy, -haloalkylthio, -alkylsulfonyl) were prepared 3,4-Cl(F<sub>3</sub>C)C<sub>6</sub>H<sub>3</sub>NH<sub>2</sub> and Et<sub>3</sub>N in MePh were added to Me<sub>2</sub>CPhCOCl in MePh at 0°, and the reaction mixture was refluxed for 2 h to give I (Ar = Ph, R<sup>1</sup> = H, R<sup>2</sup> = R<sup>3</sup> = Me, X = Cl, Y = F<sub>3</sub>C) (II). II and I showed superior herbicidal effect and equally good selectivity in crop plants, compared to two similar known herbicides.

IT 147631-58-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 147631-58-1 CAPLUS

CN 2-Thiopheneacetamide, N-[3-chloro-4-(trifluoromethyl)phenyl]-  
α,α-dimethyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



*ohay*

L4 ANSWER 107 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:651364 CAPLUS

DOCUMENT NUMBER: 117:251364

TITLE: Preparation of [(carboxybiphenyl)methyl]pyridones, -pyrimidones, and related compounds as angiotensin II receptor blockers

INVENTOR(S): Bantick, John Raymond; McInally, Thomas; Tinker, Alan Charles; Hirst, Simon Christopher

PATENT ASSIGNEE(S): Fisons PLC, UK

SOURCE: Eur. Pat. Appl., 39 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 500297	A1	19920826	EP 1992-301283	19920217
R: PT				
ZA 9201022	A	19930127	ZA 1992-1022	19920212
CN 1068109	A	19930120	CN 1992-101623	19920214

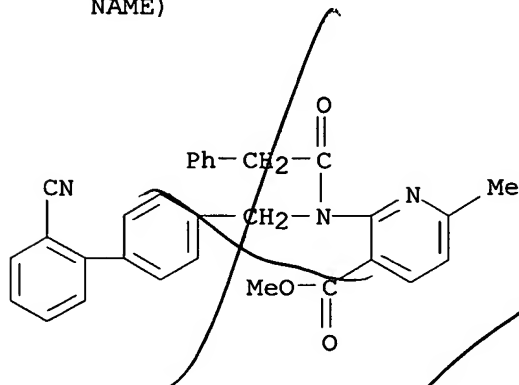
6-butyl-3-cyano-2(1H)-pyridone and Me 4'-bromomethyl-1,1'-biphenyl-2-carboxylate were coupled using NaH in DMF; the product was saponified with LiOH followed by conversion to the dicyclohexylamine salt II.

IT 144458-61-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as intermediate for angiotensin II receptor blocker)

RN 144458-61-7 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-[[[2'-cyano[1,1'-biphenyl]-4-yl)methyl](phenylacetyl)amino]-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 108 OF 174

ACCESSION NUMBER:

CAPLUS COPYRIGHT 2005 ACS on STN

1992:607151 CAPLUS

DOCUMENT NUMBER:

117:207151

TITLE:

Preparation of heteroacetic acid amide derivatives as agrochemical microbicides.

INVENTOR(S):

Ishikawa, Hiromichi; Taniguchi, Masakazu; Kajikawa, Kazuo

PATENT ASSIGNEE(S):

Hokko Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

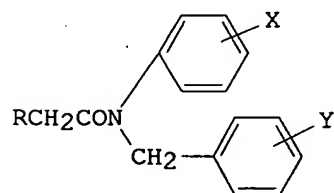
FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04145067	A2	19920519	JP 1990-265231	19901004
PRIORITY APPLN. INFO.:			JP 1990-265231	19901004
OTHER SOURCE(S):	MARPAT	117:207151		

GI



I

AB Heteroacetic acid amide derivs. I (X, Y = H, halo, lower alkyl; R = piperidino, methylpiperidino, dimethylpiperidino, hexamethyleneimino, pyrazolyl, imidazolyl, triazolyl) are prepared as agrochem. microbicides. I control downy mildew, powdery mildew, rust, etc., in fruit trees, vegetables, and cereals. Thus, 20.1 g N-phenylimidazole acetic acid amide and 16.1 g p-chlorobenzyl chloride was mixed with acetonitrile and K2CO3,

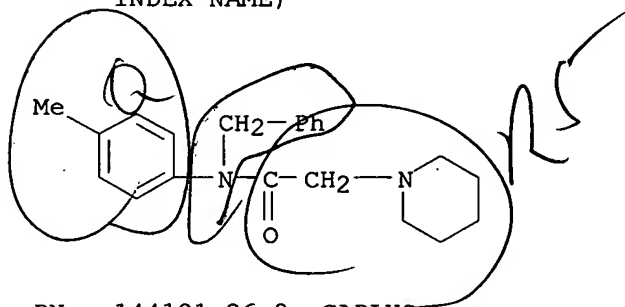
and stirred at 80° for 2 h to give 32.5 g I (R = imidazolyl, X = H, Y = 4-chloro; II). II 20, K alkylbenzenesulfonate 3, polyoxyethylene nonylphenyl ether 5, and china clay 72 parts were mixed to give a wettable powder. II, at 100 ppm, totally controlled cucumber downy mildew induced by Pseudoperonospora cubensis without damaging cucumber, vs. less effect for chlorothalonil.

IT 24853-49-4P 144121-36-8P 144121-37-9P  
 144121-38-0P 144121-39-1P 144121-40-4P  
 144121-41-5P 144121-42-6P 144121-43-7P  
 144121-44-8P 144121-45-9P 144121-46-0P  
 144121-47-1P 144121-48-2P 144121-49-3P  
 144121-50-6P 144121-51-7P 144121-52-8P  
 144121-53-9P 144121-54-0P 144121-55-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of, as agrochem. microbicide)

RN 24853-49-4 CAPLUS

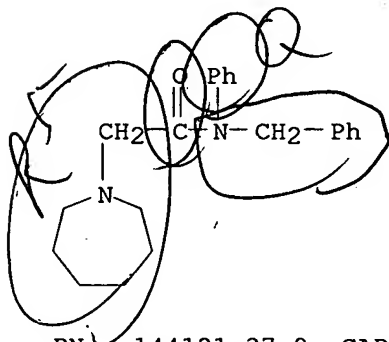
CN 1-Piperidineacetamide, N-(4-methylphenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



Yes (1)

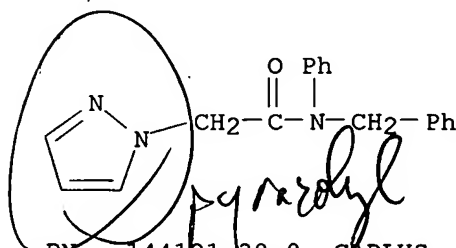
RN 144121-36-8 CAPLUS

CN 1H-Azepine-1-acetamide, hexahydro-N-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 144121-37-9 CAPLUS

CN 1H-Pyrazole-1-acetamide, N-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

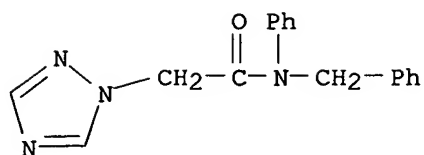


RN 144121-38-0 CAPLUS

CN 1H-1,2,4-Triazole-1-acetamide, N-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

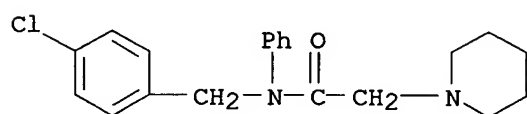
Yes (2)

Yes



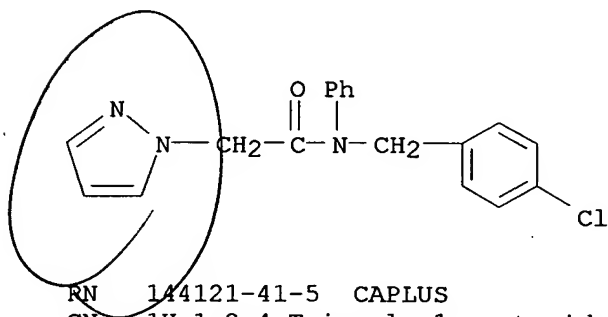
RN 144121-39-1 CAPLUS

CN 1-Piperidineacetamide, N-[(4-chlorophenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 144121-40-4 CAPLUS

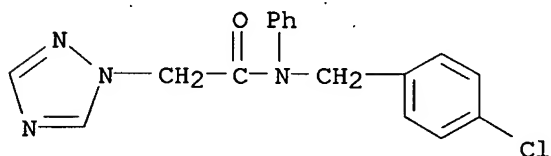
CN 1H-Pyrazole-1-acetamide, N-[(4-chlorophenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)



Yes (3)

RN 144121-41-5 CAPLUS

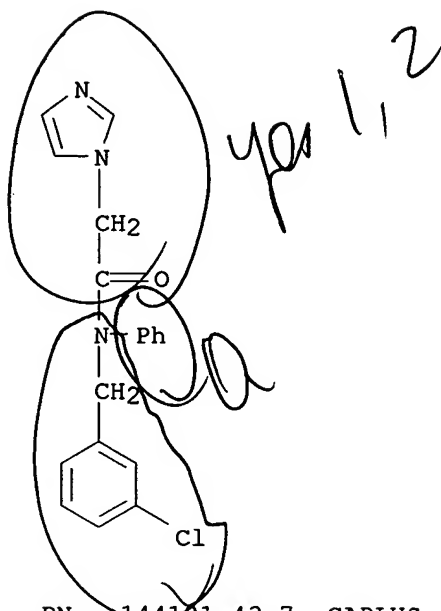
CN 1H-1,2,4-Triazole-1-acetamide, N-[(4-chlorophenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 144121-42-6 CAPLUS

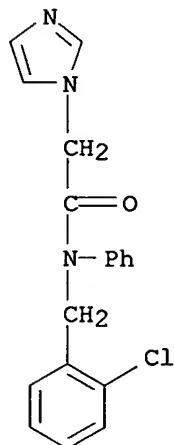
CN 1H-Imidazole-1-acetamide, N-[(3-chlorophenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)





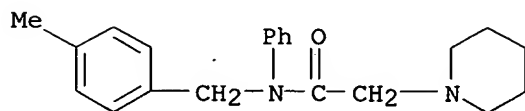
RN 144121-43-7 CAPLUS

CN 1H-Imidazole-1-acetamide, N-[(2-chlorophenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)



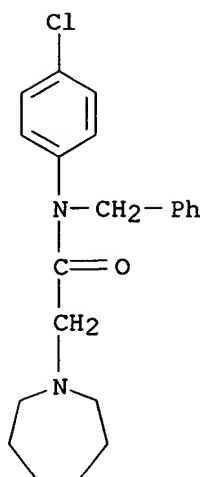
RN 144121-44-8 CAPLUS

CN 1-Piperidineacetamide, N-[(4-methylphenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)

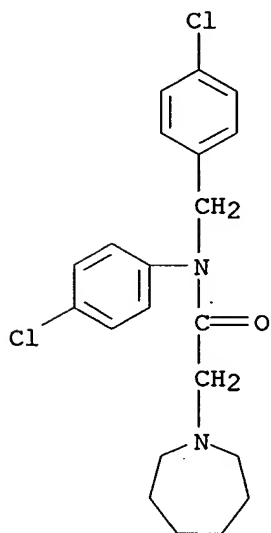


RN 144121-45-9 CAPLUS

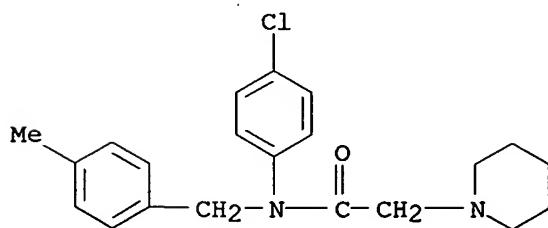
CN 1H-Azepine-1-acetamide, N-(4-chlorophenyl)hexahydro-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 144121-46-0 CAPLUS  
 CN 1H-Azepine-1-acetamide, N-(4-chlorophenyl)-N-[(4-chlorophenyl)methyl]hexahydro- (9CI) (CA INDEX NAME)

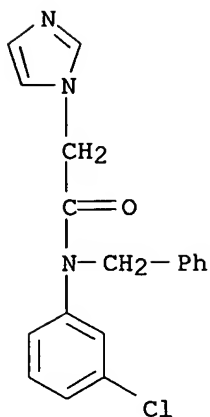


RN 144121-47-1 CAPLUS  
 CN 1-Piperidineacetamide, N-(4-chlorophenyl)-N-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 144121-48-2 CAPLUS  
 CN 1H-Imidazole-1-acetamide, N-(3-chlorophenyl)-N-(phenylmethyl)- (9CI) (CA

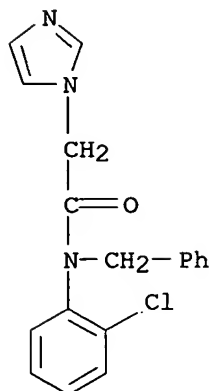
INDEX NAME)



Yes 2

RN 144121-49-3 CAPLUS

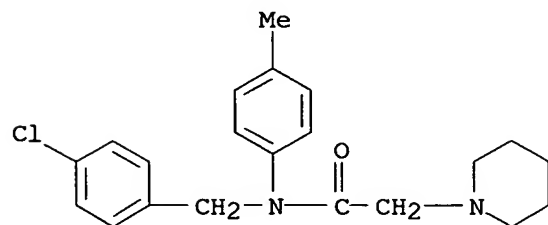
CN 1H-Imidazole-1-acetamide, N-(2-chlorophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



Yes 2

RN 144121-50-6 CAPLUS

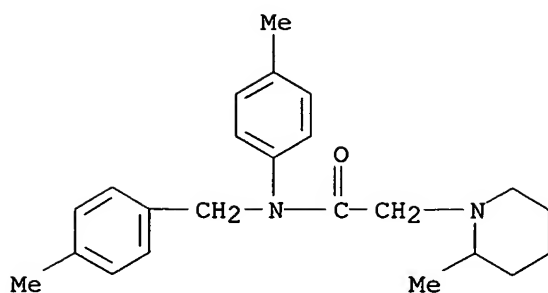
CN 1-Piperidineacetamide, N-[(4-chlorophenyl)methyl]-N-(4-methylphenyl)- (9CI) (CA INDEX NAME)



Yes 1

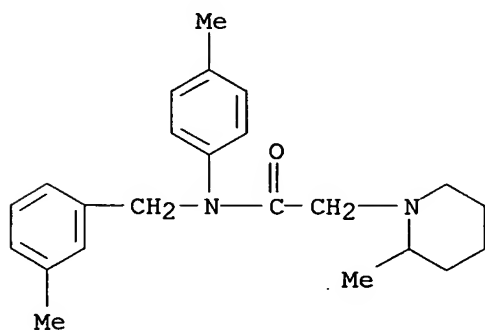
RN 144121-51-7 CAPLUS

CN 1-Piperidineacetamide, 2-methyl-N-(4-methylphenyl)-N-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



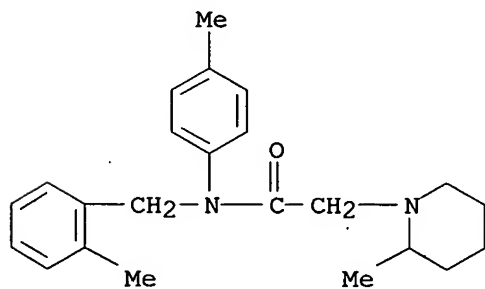
RN 144121-52-8 CAPLUS

CN 1-Piperidineacetamide, 2-methyl-N-(4-methylphenyl)-N-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



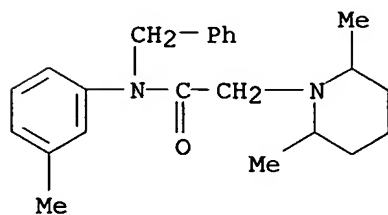
RN 144121-53-9 CAPLUS

CN 1-Piperidineacetamide, 2-methyl-N-(4-methylphenyl)-N-[(2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

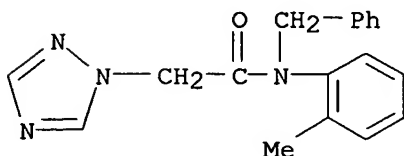


RN 144121-54-0 CAPLUS

CN 1-Piperidineacetamide, 2,6-dimethyl-N-(3-methylphenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 144121-55-1 CAPLUS  
 CN 1H-1,2,4-Triazole-1-acetamide, N-(2-methylphenyl)-N-(phenylmethyl)- (9CI)  
 (CA INDEX NAME)



L4 ANSWER 109 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1991:164819 CAPLUS  
 DOCUMENT NUMBER: 114:164819  
 TITLE: Preparation and formulation of ureidoalkanamides, peptides, and analogs as cholecystokinin receptor antagonists  
 INVENTOR(S): Bourzat, Jean Dominique; Capet, Marc; Cotrel, Claude; Guyon, Claude; Manfre, Franco; Roussel, Gerard  
 PATENT ASSIGNEE(S): Rhone-Poulenc Sante, Fr.  
 SOURCE: Eur. Pat. Appl., 28 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 397556	A1	19901114	EP 1990-401218	19900509
EP 397556	B1	19931020		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2646847	A1	19901116	FR 1989-6250	19890512
FR 2646847	B1	19910712		
AT 96146	E	19931115	AT 1990-401218	19900509
ES 2060097	T3	19941116	ES 1990-401218	19900509
CA 2016439	AA	19901112	CA 1990-2016439	19900510
JP 03056453	A2	19910312	JP 1990-120182	19900511
US 5223529	A	19930629	US 1990-522137	19900511
PRIORITY APPLN. INFO.:			FR 1989-6250	A 19890512
			EP 1990-401218	A 19900509

OTHER SOURCE(S): CASREACT 114:164819; MARPAT 114:164819

AB R3CONHZCONR1Ph [I; R1 = CHR8CO2R4, CH2CONR5R6, phenylalkyl, (un)substituted Ph; R3 = 1- or 2-naphthyl, 2- or 3-indolyl, (un)substituted PhNH; R4 = H, (cyclo)alkyl, Ph, phenylalkyl, etc.; R5, R6 = alkyl; NR5R6 = (alkyl)pyrrolidino; R8 = H, alkyl, Ph; Z = CH2, CH2CH2, CHR7; R7 = alkyl, Ph, PhCH2, etc.] were prepared Thus, PhNH2 was condensed with BrCH2CO2CMe3 and the product condensed with ClCH2COCl to give ClCH2CONPhCO2CMe3 which was condensed with K phthalimide and the product hydrozinolized to give H2NCH2CONPhCH2CO2CMe3. The latter was condensed with 3-MeC6H4NCO to give 3-MeC6H4NHCONHCH2CONPhCH2CO2CMe3. I have IC50 ≤ 103 nM for cholecystokinin receptor binding.

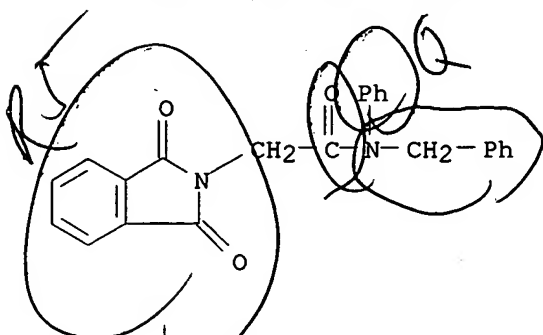
IT 133115-35-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrazinolysis of, in preparation of cholecystokinin receptor antagonist)

RN 133115-35-2 CAPLUS

CN 2H-Isoindole-2-acetamide, 1,3-dihydro-1,3-dioxo-N-phenyl-N-(phenylmethyl)-  
(9CI) (CA INDEX NAME)



L4 ANSWER 110 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1991:81260 CAPLUS  
DOCUMENT NUMBER: 114:81260  
TITLE: Preparation of (acylamino)benzoic acid derivatives as  
reverse transcriptase inhibitors  
INVENTOR(S): Fukushima, Daikichi; Okuyama, Shigehiro; Miyamoto,  
Tsumoru  
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02218654	A2	19900831	JP 1988-256668	19881012
PRIORITY APPLN. INFO.:			JP 1988-256668	19881012

OTHER SOURCE(S): MARPAT 114:81260

GI For diagram(s), see printed CA Issue.

AB The title compds. (I; R = Q; R1 = H, C1-8 alkyl or alkoxy, halo, CF3; 1 = 1-5; ring A, B = 4- to 10-membered carbocycle or heterocycle; Y = OZ1O, Z1O, Z1, where Z1 = C1-8 alkylene; R2 = H, C1-4 alkyl or alkoxy, halo, CF3, C2-5 alkanoyl; m = 1-4; Z = single bond, C1-6 alkylene, C2-6 alkenylene; R3 = H, C1-4 alkyl, Ph, phenylalkyl; R4 = H, C1-4 alkyl or alkoxy, halo, CF3, OH, NO2), useful for treatment or prophylaxis of retrovirus infection, e.g. AIDS, are prepared by amidation of I (R = H) with QOH. Thus, 140 mg 3-[(4-pentylphenoxy)propoxy]benzoic acid was stirred 30 min at room temperature with excess (ClCO)2 and after concentration in vacuo

was

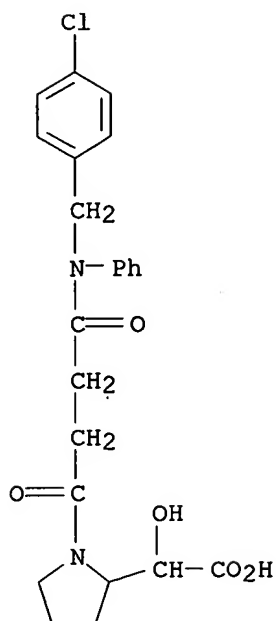
stirred overnight with 82 mg 5-chloroanthranilic acid Et ester in Cl2CH2 in the presence of Et3N to give benzoate [II; R5 = Et, R6 = PhCCH2)3O] which was saponified with 2N ag. NaOH in EtOH to give 65 mg II [R5 = H, R6 = Ph(CH2)3O]. A total of 82 I were prepared and 13 I were in vitro tested for inhibiting reverse transcriptase of mouse leukemia; I exhibited IC50 values of 0.7 to 3.9  $\mu$ M.

IT 131820-16-1P

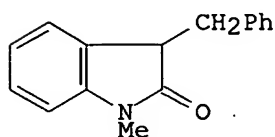
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as reverse transcriptase inhibitor)

RN 131820-16-1 CAPLUS

CN Benzoic acid, 5-chloro-2-[[1-oxo-3-[4-(4-phenylbutyl)phenyl]-2-propenyl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)



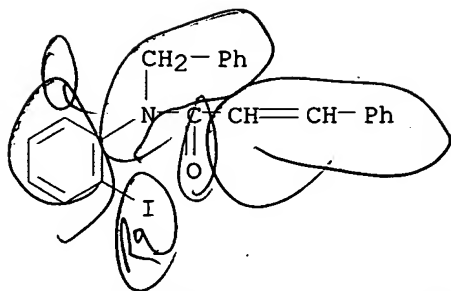
L4 ANSWER 112 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1989:497034 CAPLUS  
 DOCUMENT NUMBER: 111:97034  
 TITLE: Synthesis of oxindoles by radical cyclization  
 AUTHOR(S): Bowman, W. Russell; Heaney, Harry; Jordan, Benjamin M.  
 CORPORATE SOURCE: Dep. Chem., Univ. Technol., Loughborough/Leics., LE11 3TU, UK  
 SOURCE: Tetrahedron Letters (1988), 29(50), 6657-60  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 111:97034  
 GI



I

1, 2, 3, 4

AB Oxindoles are readily synthesized by intramol. addition of aryl radicals to the  $\alpha$ -position of  $\alpha,\beta$ -unsatd. N-alkylamides. Thus, o-IC<sub>4</sub>H<sub>4</sub>NMeCOCH:CHPh was treated with Bu<sub>3</sub>SnH and AIBN to give the oxindole I in 33% yield.  
 IT **122101-01-3P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and radical cyclization of, oxindole derivative from)  
 RN 122101-01-3 CAPLUS  
 CN 2-Propenamide, N-(2-iodophenyl)-3-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



yes 1, 2, 3, 4

L4 ANSWER 113 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:192328 CAPLUS

DOCUMENT NUMBER: 110:192328

TITLE: Rhodium(I)-catalyzed asymmetric hydrogenation of imines

AUTHOR(S): Kang, Guo Jun; Cullen, William R.; Fryzuk, Michael D.; James, Brian R.; Kutney, James P.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SOURCE: Journal of the Chemical Society, Chemical Communications (1988), (22), 1466-7  
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:192328

AB High-pressure hydrogenation of  $\text{RC}_6\text{H}_4\text{CMe:NCH}_2\text{Ph}$  ( $\text{R} = \text{H}$ , *o*- and *p*-MeO) in the presence of a catalyst prepared from chloronorbornadienylnorbornadienylrhodium dimer and (R)-(+)-Ph<sub>2</sub>PCHR<sub>1</sub>CH<sub>2</sub>PPh<sub>2</sub> ( $\text{R}_1 = \text{cyclohexyl}$ ) in 1:1 C<sub>6</sub>H<sub>6</sub>-MeOH containing KI gave 90-100% (S)- $\text{RC}_6\text{H}_4\text{CHMeNHCH}_2\text{Ph}$  in 60-91% enantiomeric excess.

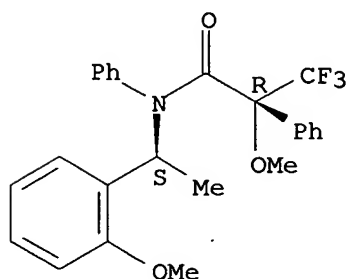
IT **120343-47-7P 120343-48-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 120343-47-7 CAPLUS

CN Benzeneacetamide,  $\alpha$ -methoxy-N-[1-(2-methoxyphenyl)ethyl]-N-phenyl- $\alpha$ -(trifluoromethyl)-, [R-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 120343-48-8 CAPLUS

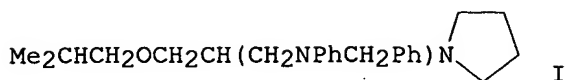
CN Benzeneacetamide,  $\alpha$ -methoxy-N-[1-(4-methoxyphenyl)ethyl]-N-phenyl- $\alpha$ -(trifluoromethyl)-, [R-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



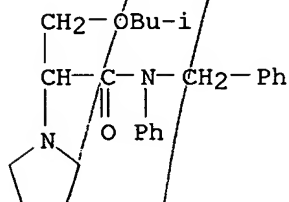
FR 2378024	A1	19780818	FR 1977-2058	19770125
FR 2378024	B1	19790511		
PRIORITY APPLN. INFO.:			IL 1973-41619	A 19730226
			FR 1977-2058	A 19770125

GI

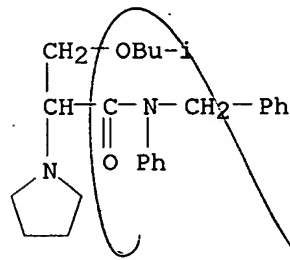


AB The title compound I was prepared by treating BrCH<sub>2</sub>CHBrCO<sub>2</sub>Et with Me<sub>2</sub>CHCH<sub>2</sub>OH, treating Me<sub>2</sub>CHCH<sub>2</sub>OCH<sub>2</sub>CHBrCO<sub>2</sub>Et with pyrrolidine, Grignard reaction with PhNHCH<sub>2</sub>Ph, and reduction of the amide function. I is superior to amiodarone in the treatment of angina pectoris.

IT **68099-85-4P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and hydride reduction of)  
 RN 68099-85-4 CAPLUS  
 CN 1-Pyrrolidineacetamide, α-[(2-methylpropoxy)methyl]-N-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT **79276-57-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 79276-57-6 CAPLUS  
 CN 1-Pyrrolidineacetamide, α-[(2-methylpropoxy)methyl]-N-phenyl-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



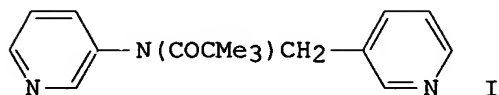
● HCl

L4 ANSWER 125 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1981:497849 CAPLUS  
 DOCUMENT NUMBER: 95:97849  
 TITLE: Heterocyclic compounds with fungicidal, herbicidal and plant growth regulating properties

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.,  
Neth.  
SOURCE: Neth. Appl., 48 pp.  
CODEN: NAXXAN  
DOCUMENT TYPE: Patent  
LANGUAGE: Dutch  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 8004078	A	19810121	NL 1980-4078	19800716
CA 1231710	A1	19880119	CA 1980-353294	19800603
BE 884340	A1	19810116	BE 1980-201427	19800716
DK 8003077	A	19810120	DK 1980-3077	19800716
DK 163907	B	19920421		
DK 163907	C	19920921		
FI 8002258	A	19810120	FI 1980-2258	19800716
FI 76792	B	19880831		
FI 76792	C	19881212		
NO 8002135	A	19810120	NO 1980-2135	19800716
NO 164451	B	19900702		
NO 164451	C	19901010		
SE 8005190	A	19810120	SE 1980-5190	19800716
SE 452544	B	19871207		
SE 452544	C	19880317		
AU 8060440	A1	19810122	AU 1980-60440	19800716
AU 536746	B2	19840524		
FR 2461457	A1	19810206	FR 1980-15679	19800716
FR 2461457	B1	19841116		
JP 56016469	A2	19810217	JP 1980-96326	19800716
JP 02004566	B4	19900129		
BR 8004436	A	19810224	BR 1980-4436	19800716
GB 2056974	A	19810325	GB 1980-23292	19800716
GB 2056974	B2	19840229		
DE 3026926	A1	19810430	DE 1980-3026926	19800716
ES 493416	A1	19810516	ES 1980-493416	19800716
ZA 8004285	A	19810624	ZA 1980-4285	19800716
DD 154468	C	19820324	DD 1980-222670	19800716
AT 8003691	A	19820715	AT 1980-3691	19800716
AT 369950	B	19830210		
HU 26548	O	19830928	HU 1980-1776	19800716
HU 186300	B	19850729		
RO 84716	P	19840717	RO 1980-101724	19800716
IL 60614	A1	19840831	IL 1980-60614	19800716
CH 647649	A	19850215	CH 1980-5467	19800716
SU 1186073	A3	19851015	SU 1980-2950207	19800716
CS 266307	B2	19891213	CS 1980-5048	19800716
GB 2124615	A1	19840222	GB 1983-15625	19830607
GB 2124615	B2	19840718		
PRIORITY APPLN. INFO.:			GB 1979-25164	A 19790719
			GB 1980-23292	A3 19800716

GI



AB RR1NCHR2R3 (one of R, R2 = optionally substituted 6-membered heterocycle containing 1-2 N and the other is the same or optionally substituted Ph; R1 =

acyl; R3 = H, alkyl) were prepared Thus 3-(3-pyridyliminomethyl)pyridine was reduced to the amine and acylated with Me3CCOCl to give I. At 1 kg/ha on barley I gave > 80% protection against Erisyphe graminis. I also had herbicidal activity.

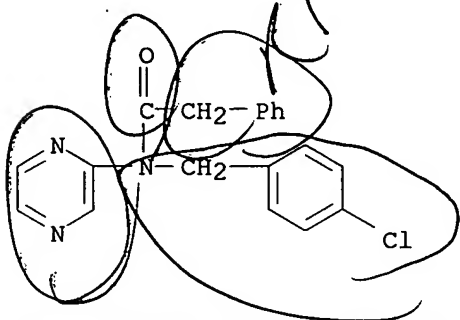
IT 78675-71-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and fungicidal activity of)

RN 78675-71-5 CAPLUS

CN Benzeneacetamide, N-[(4-chlorophenyl)methyl]-N-pyrazinyl- (9CI) (CA INDEX NAME)



yes 1, 2  
not 3, 4

L4 ANSWER 126 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1981:406772 CAPLUS

DOCUMENT NUMBER: 95:6772

TITLE: Medicinal derivatives of 2-benzoyl-4-nitro anilides

INVENTOR(S): Mouzin, Gilbert; Cousse, Henri

PATENT ASSIGNEE(S): Fabre, Pierre, S. A., Fr.

SOURCE: Eur. Pat. Appl., 32 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

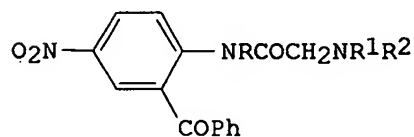
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 22017	A1	19810107	EP 1980-400942	19800624
EP 22017	B1	19820505		
R: AT, BE, CH, DE, GB, IT, LU, NL, SE				
FR 2459793	A1	19810116	FR 1979-16213	19790625
FR 2459793	B1	19830909		
AU 8059531	A1	19810108	AU 1980-59531	19800623
AU 536228	B2	19840503		
ES 493256	A1	19810416	ES 1980-493256	19800623
ZA 8003721	A	19810729	ZA 1980-3721	19800623
AT 960	E	19820515	AT 1980-400942	19800624
JP 56008353	A2	19810128	JP 1980-86399	19800625
CA 1141380	A1	19830215	CA 1980-354714	19800625

PRIORITY APPLN. INFO.:

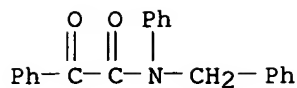
FR 1979-16213 A 19790625  
EP 1980-400942 A 19800624

OTHER SOURCE(S): CASREACT 95:6772

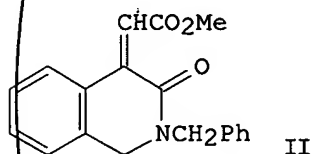
GI



I



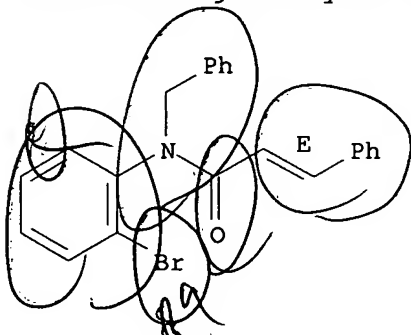
L4 ANSWER 134 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1979:575155 CAPLUS  
 DOCUMENT NUMBER: 91:175155  
 TITLE: Reactions and syntheses with organometallic compounds.  
 X. The intramolecular cyclization using arylpalladium  
 complexes for generation of nitrogen-heterocycles  
 AUTHOR(S): Mori, Miwako; Ban, Yoshio  
 CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, Japan  
 SOURCE: Tetrahedron Letters (1979), (13), 1133-6  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 91:175155  
 GI



AB 2-BrC6H4(CH2)nN(CH2Ph)COR (I; n = 1, R = cis-CH:CHCO2Me), prepared by reaction of 2-BrC6H4CH2NHCH2Ph with maleic anhydride, underwent exo cyclization in PhCN containing Pd(OAc)2/PPh3 at 125° to give 47.3% of an isomeric mixture of isoquinolinones II. I [n = 0, R = cis-CH:CHCO2Me, trans-CH:CHPh, CH(CO2Et)CH2CH:CHCO2Me] underwent similar Pd-catalyzed exo cyclizations to give N heterocycles.

IT 71687-75-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of, palladium-catalyzed)  
 RN 71687-75-7 CAPLUS  
 CN 2-Propenamide, N-(2-bromophenyl)-3-phenyl-N-(phenylmethyl)-, (E)- (9CI)  
 (CA INDEX NAME)

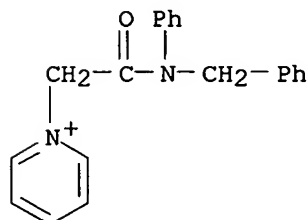
Double bond geometry as shown.



Yes 12 34

L4 ANSWER 135 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1979:551080 CAPLUS  
 DOCUMENT NUMBER: 91:151080  
 TITLE: New antiarrhythmic agents. 2. Amide alkyl  
 $\alpha$ -amino xylidides  
 AUTHOR(S): McMaster, Paul D.; Byrnes, Eugene W.; Feldman, Hal S.;  
 Takman, Bertil H.; Tenthorey, Paul A.

L4 ANSWER 146 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1975:514139 CAPLUS  
 DOCUMENT NUMBER: 83:114139  
 TITLE: N-Substituted isatins from phenylnitrones of glyoxyl anilides  
 AUTHOR(S): Heinisch, L.  
 CORPORATE SOURCE: Zentralinst. Mikrobiol. Exp. Ther., DAW, Jena, Ger. Dem. Rep.  
 SOURCE: Journal fuer Praktische Chemie (Leipzig) (1975), 317(3), 435-47  
 CODEN: JPCEAO; ISSN: 0021-8383  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 83:114139  
 GI For diagram(s), see printed CA Issue.  
 AB Isatins I (X1 = O, R = Me, Et, Pr, Bu, CH2Ph, Ph) were prepared by treating PhNHR with ClCH2COCl, treating PhNRCOCH2Cl with pyridine, treating the pyridinium salts II (X = O, X = Cl) with p-Me2NC6H4NO, and hydrolyzing PhNRCOCH:N(O)C6H4NMe2-p with acid. I (X1 = S, R = Me, Et, Ph) were similarly obtained from the pyridine salts II (X1 = S, X = Cl, H2PO2S2, PO2S), prepared from PhNRCSCH2Cl, which were prepared by treating PhNRCOCH2Cl with P2S5.  
 IT **57988-97-3P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with nitrosodimethylaniline)  
 RN 57988-97-3 CAPLUS  
 CN Pyridinium, 1-[2-oxo-2-[phenyl(phenylmethyl)amino]ethyl]-, chloride (9CI)  
 (CA INDEX NAME)



● Cl<sup>-</sup>

L4 ANSWER 147 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1974:132977 CAPLUS  
 DOCUMENT NUMBER: 80:132977  
 TITLE: Rearrangement reaction of N-alkyl-α-haloacetanilides with Grignard reagents. Synthesis of indole-3-acetic acid  
 AUTHOR(S): Mori, Miwako; Nishimura, Shigeko; Ban, Yoshio  
 CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, Japan  
 SOURCE: Tetrahedron Letters (1973), (49), 4951-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB Refluxing ethereal PhMeNCOCH2Br (I) and excess EtMgBr containing a catalytic

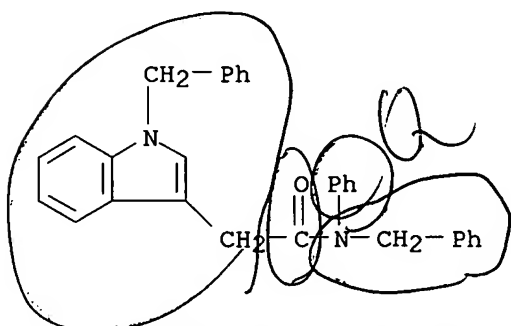
amount of  $\text{NiCl}_2(\text{PPh}_3)_2$  for 24 hr gave 38.1%  $\text{PhNMe}(\text{CH}_2\text{CO})_2\text{NMePh}$  (II) and 27.1%  $(\text{PhNMeCOCH}_2)_2$  (III) via an enamine and 8.1%  $\text{PhNMeAc}$ . I with  $\text{EtMgBr}$  in THF at  $30^\circ$  rapidly gave II and at  $-10^\circ$  gave III.  $\text{PhNMeCOCH}_2\text{Cl}$  and  $\text{PhCH}_2\text{NPhCOCH}_2\text{Br}$  reacted similarly.  $\text{PhNHCOCH}_2\text{Br}$  gave  $(\text{PhNHCOCH}_2)_2$  quant. I in THF with  $\text{PhMgBr}$  or  $\text{Mg}$  gave II. Heating  $\text{PhCH}_2\text{NPh}(\text{CH}_2\text{CO})_2\text{NPhCH}_2\text{Ph}$  with  $\text{ZnCl}_2$  gave the anilide (IV) which on debenzoylation and acid hydrolysis gave indole-3-acetic acid.

IT 52190-17-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 52190-17-7 CAPLUS

CN 1H-Indole-3-acetamide, N-phenyl-N,1-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



*Handwritten signature*

L4 ANSWER 148 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:526414 CAPLUS

DOCUMENT NUMBER: 79:126414

TITLE: Potential local anesthetics. IX. Synthesis of diethylamino-, morpholino-, or piperidino-N-(substituted benzyl)acetanilides

AUTHOR(S): Patel, P. B.; Trivedi, J. J.

CORPORATE SOURCE: Chem. Lab., Smt. Bhikhuben Chandulal Jalundhwala Sci. Coll., Cambay, India

SOURCE: Journal of the Indian Chemical Society (1973), 50(4), 287-9

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB About 40 title compds. I ( $R = \text{H}, o\text{-Me}, p\text{-Me}, o\text{-Cl}, p\text{-Cl}, 3,4\text{-Me}_2, 2,4\text{-Me}_2$ ;  $R_1 = \text{H}, o\text{-Me}, m\text{-Me}, p\text{-Me}, o\text{-MeO}, p\text{-MeO}, m\text{-Cl}$ ;  $R_2 = R_3 = \text{Et}, R_2R_3 = (\text{CH}_2)_5, \text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2$ ) were prepared by treating benzylamines with  $\text{ClCH}_2\text{COCl}$  and the resulting  $\alpha$ -chloro-N-benzylacetanilides with  $\text{Et}_2\text{NH}$ , morpholine, or piperidine. I ( $R = \text{H}, R_1 = p\text{-Me}, R_2R_3 = \text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2$ ) was twice as active as lignocaine as a surface and intradermal anaesthetic.

IT 27241-96-9P 27241-97-0P 27241-99-2P

27242-00-8P 27291-87-8P 27291-88-9P

27291-90-3P 27291-91-4P 50400-90-3P

50400-91-4P 50400-92-5P 50400-93-6P

50400-96-9P 50400-97-0P 50625-71-3P

50625-72-4P 50625-73-5P 50625-74-6P

50625-75-7P 50625-76-8P 50625-77-9P

50625-78-0P 50798-88-4P 50798-89-5P

50798-91-9P 50798-92-0P 50798-93-1P

50886-50-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 27241-96-9 CAPLUS

CN 4-Morpholineacetamide, N-(3-methylphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

isomer observed was that with the o-substituted benzene ring trans to O (except for formanilides). However, rotation around the N-benzene bond is preceded by rotation around the carbonyl-N bond to give the activated state. Variations in barrier height from compound to compound are rationalized in terms of steric and electronic factors.

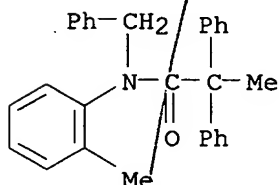
IT **20643-11-2**

RL: PRP (Properties)

(potential barrier to rotation in)

RN 20643-11-2 CAPLUS

CN o-Propionotoluidide, N-benzyl-2,2-diphenyl- (8CI) (CA INDEX NAME)



L4 ANSWER 152 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:501818 CAPLUS

DOCUMENT NUMBER: 71:101818

TITLE: Synthesis and central nervous system depressant activity of new piperazine and related derivatives. III

AUTHOR(S): Petigara, R. B.; Deliwala, Chimanlal; Mandrekar, S. S.; Dadkar, N. K.; Sheth, U. K.

CORPORATE SOURCE: Haffkine Inst., Bombay, India

SOURCE: Journal of Medicinal Chemistry (1969), 12, 865-70  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

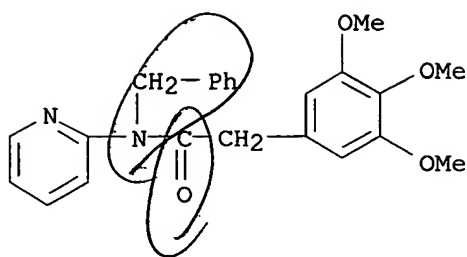
AB Several N1,N4-disubstituted piperazine derivs., in which N1-substituents are 3,4,5-trimethoxy-benzoylacetyl, 3,4,5-trimethoxycinnamoyl or -hydrocinnamoyl, 3,4,5-trimethoxyphenylpropyl, and 3,4,5-trimethoxybenzoyl-alkyl and N4-substituents are benzyl, m-methyl- or p-tert-butylbenzyl, p-chloro- $\alpha$ -phenylbenzyl, Ph, chloro-, fluoro-, or methoxyphenyl, tolyl,  $\alpha,\alpha,\alpha$ -trifluorotolyl, 2-pyridyl, 2-pyrimidinyl, or 2-thiazolyl groups, have been synthesized. Analogous compds. with other alkyl and heterocyclic amines in place of piperazine have also been synthesized. All these compds. have been screened for CNS activity. A few of these compds. exhibited significant central nervous system (CNS) depressant activity. The 3,4,5-trimethoxyphenyl moiety was the most essential for CNS activity as stepwise omission of the methoxy groups of most active compds. resulted in loss of activity.

IT **23771-22-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 23771-22-4 CAPLUS

CN Acetamide, N-benzyl-N-2-pyridyl-2-(3,4,5-trimethoxyphenyl)-, monohydrobromide (8CI) (CA INDEX NAME)



● HBr

ya 1 2 ✓

L4 ANSWER 153 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:96715 CAPLUS

DOCUMENT NUMBER: 70:96715

TITLE: Acylation of nitrogen heterocycles under the conditions of the Schotten-Baumann reaction. I. Benzimidazoles

AUTHOR(S): Ben-Ishai, Dov; Babad, E.; Bernstein, Z.

CORPORATE SOURCE: Technion-Israel Inst. Technol., Haifa, India

SOURCE: Israel Journal of Chemistry (1968), 6(5), 551-67

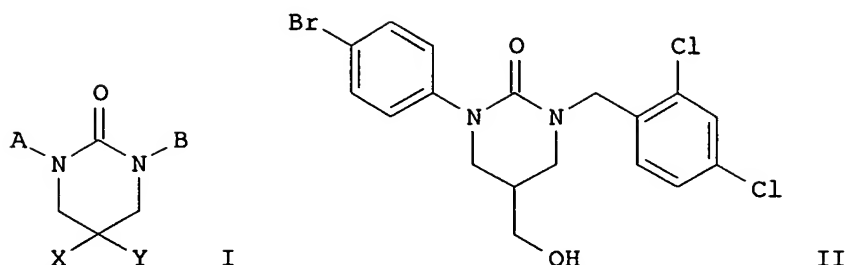
CODEN: ISJCAT; ISSN: 0021-2148

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1-(R-Substituted)-2-(R1-substituted)benzimidazoles (I) are acylated to give phenylenediamines o-RN(COR1)-C6H4NHCOR2 (II); 1-(R-substituted)-2-(R1-substituted)-3-(R2-substituted)-2-hydroxybenzimidazolines (III) and 1-(R-substituted)-3-(R1-substituted)-2-benzimidazolones (IV) are also prepared. Thus, 0.005 mole I (R1 = H) are treated with 0.0075 mole ClCO2CH2Ph in EtOAc in the presence of N NaHCO3 to give N-phenethyl-N'-formyl-N'-carbobenzoxy-o-phenylenediamine, m. 85-6°, and the following II (R1 = H, R2 = OCH2Ph) (R and m.p. given): PhCH2, 108-9°; p-O2NC6H4CH2, 107-8°; Ph, 130-1°; CH2CH2CONH2, 178-9°; CH2CH2CO2H, 103-4°; CH2CO2CH2Ph, 97-9°; CH2CONH2, 181-2°; CH2CO2H, 144-5°; CH2CH2OBz, 88-90°; CH2CH2SCH2Ph, -; and p-O2N-C6H4, 158-9°. Similarly prepared are the following II (R = PhCH2, R1 = H) (R2 and m.p. given): OMe, 117-18°; OEt, 132-3°; and OBU-iso, 108-9°; the following II (R1 = H, R2 = Ph) (R and m.p. given): PhCH2CH2, 164-5°; PhCH2, 118-19°; p-O2NC6H4CH2, 153-4°; Ph, 131-2°; p-O2NC6H4, 106-8°; BzOCH2CH2, 146-7°; EtO2CCH2, 107-8°; and H2NCOCH2, 174-5°; the following II (R = PhCH2CH2, R1 = H) (R2 and m.p. given): p-O2NC6H4, 134-5°; o-O2NC6H4, 159-60°; p-MeOC6H4, 80-3°; o-MeOC6H4, 118-19°; and o-tolyl, 88-9°; the following II (R = PhCH2, R1 = H) (R2 and m.p. given): p-O2NC6H4, 11-13°; o-O2NC6H4, 62-3°; p-MeOC6H4, 105-6°; o-MeOC6H4, 104°; and o-tolyl, 119-20°; the following II (R = EtO2CCH2CH2, R1 = H) (R2 and m.p. given): p-O2NC6H4, 116-18°; p-MeOC6H4, -; o-MeOC6H4, 84-5°; and o-tolyl, -; the following II (R = H2NCOCH2CH2, R1 = H) (R2 and m.p. given): p-O2NC6H4, 156-7°; o-MeOC6H4, 170-1°; and o-tolyl, 114-16°; the following II (R = PhCH2, R2 = PhCH2O) (R1 and m.p. given): Me, 127-9°; PhCH2, 101-2°; and Ph, 144-6°; and II (R = PhCH2O2C, R1 = H, R2 = Bz) (m. 107-8°), I (R = H, R1 = PhCH2) gives II (R = PhCH2O2C, R1 = Me, R2 = PhCH2O) (m. 121-2°). I (R = PhCH2O2C, R1 = H) (m. 69-70°) is treated with ClCO2CH2Ph to give III (R = R2 = PhCH2O2C, R1 = H), m. 114-16°; similarly prepared is III (R = PhCH2O2C, R1 = H, R2 = Bz) (m. 107-8°). I (R = H, R1 = PhCH2) gives III (R = R2 = PhCH2O2C, R1 = PhCH2) (m. 91-3°). III (R = R2 = PhCH2O2C, R1 = H) is treated





AB The title compds. [I; A, B = (un)substituted Ph, alkyl, heteroalkyl, etc.; X = CO<sub>2</sub>H, CO<sub>2</sub>(alkyl), SO<sub>3</sub>H, etc.; Y = H, alkyl, aryl, etc.; X and Y, taken together with the atom to which they are joined, provide a group C:ZR<sub>11</sub> (Z = CO<sub>2</sub>H, CO<sub>2</sub>(alkyl), SO<sub>3</sub>H, etc.; R<sub>11</sub> = H, alkyl, cycloalkyl, etc.)] which are α<sub>2</sub> inhibitors useful for treating diabetes and related diseases, especially Type II diabetes, were prepared E.g., a multi-step synthesis

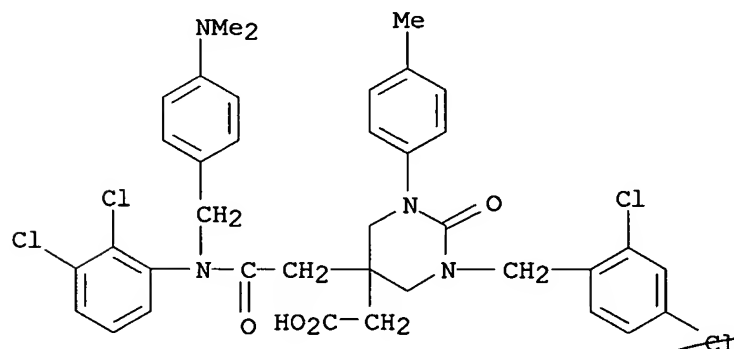
of II was given. A method is also provided for treating diabetes and related diseases, especially Type II diabetes, employing α<sub>2</sub> inhibitor I or a combination of such α<sub>2</sub> inhibitor and another antidiabetic agent such as metformin, glyburide troglitazone and/or insulin.

IT 352324-41-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of tetrahydropyrimidone inhibitors of fatty acid binding protein)

RN 352324-41-5 CAPLUS

CN 5-Pyrimidineacetic acid, 5-[2-[(2,3-dichlorophenyl)[[4-(dimethylamino)phenyl]methyl]amino]-2-oxoethyl]-1-[(2,4-dichlorophenyl)methyl]hexahydro-3-(4-methylphenyl)-2-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 56 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:488285 CAPLUS

DOCUMENT NUMBER: 135:331317

TITLE: Cathodic reduction of N-(2-iodophenyl)-N-alkylcinnamides: a novel sequential electrochemical radical cyclization and hydroxylation

AUTHOR(S): Munusamy, Raja; Samban Dhathathreyan, Kaveripatnam; Kuppasamy Balasubramanian, Kalpattu; Sivaramakrishnan Venkatachalam, Chittoor

CORPORATE SOURCE: Centre for Energy Research, SPIC Science Foundation,  
Guindy, Chennai, 600032, India

SOURCE: Journal of the Chemical Society, Perkin Transactions 2  
(2001), (7), 1154-1166  
CODEN: JCSPGI; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:331317

AB The cathodic reduction of N-(2-iodophenyl)-N-alkylcinnamamides under deaerated conditions in DMF gave 1-alkyl-3-benzylindolin-2-ones regioselectively and in the presence of oxygen yielded surprisingly 1-alkyl-3-hydroxy-3-benzylindolin-2-ones. Both these products were formed by a 5-exo-trig process in good yields. A mechanism for the formation of the products has been proposed through the use of cyclic voltammetry, coulometry and controlled-potential electrolysis as well as deuterium labeling.

IT 257630-75-4P 257630-76-5P 264618-24-8P  
264618-25-9P 370558-16-0P 370558-17-1P  
370558-37-5P

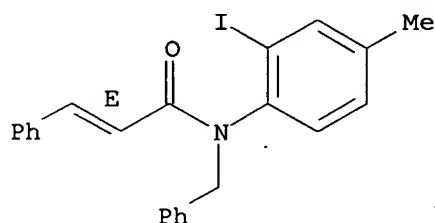
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(sequential electrochem. radical cyclization and hydroxylation of N-(2-iodophenyl)-N-alkylcinnamides)

RN 257630-75-4 CAPLUS

CN 2-Propenamide, N-(2-iodo-4-methylphenyl)-3-phenyl-N-(phenylmethyl)-, (2E)-(9CI) (CA INDEX NAME)

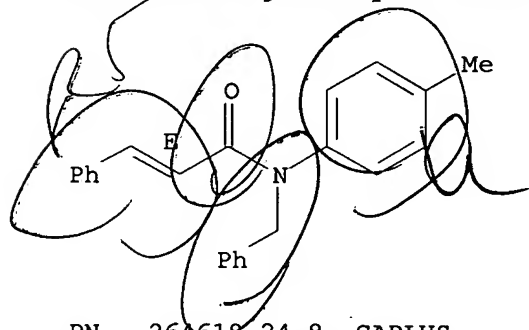
Double bond geometry as shown.



RN 257630-76-5 CAPLUS

CN 2-Propenamide, N-(4-methylphenyl)-3-phenyl-N-(phenylmethyl)-, (2E)-(9CI) (CA INDEX NAME)

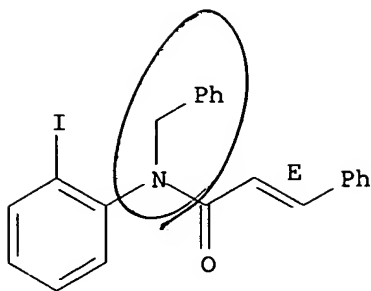
Double bond geometry as shown.



RN 264618-24-8 CAPLUS

CN 2-Propenamide, N-(2-iodophenyl)-3-phenyl-N-(phenylmethyl)-, (2E)-(9CI) (CA INDEX NAME)

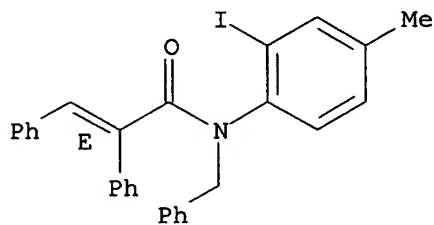
Double bond geometry as shown.



RN 264618-25-9 CAPLUS

CN Benzeneacetamide, N-(2-iodo-4-methylphenyl)-N-(phenylmethyl)-α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

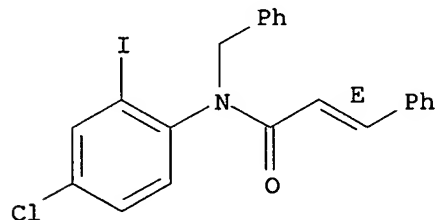
Double bond geometry as shown.



RN 370558-16-0 CAPLUS

CN 2-Propenamide, N-(4-chloro-2-iodophenyl)-3-phenyl-N-(phenylmethyl)-, (2E)- (9CI) (CA INDEX NAME)

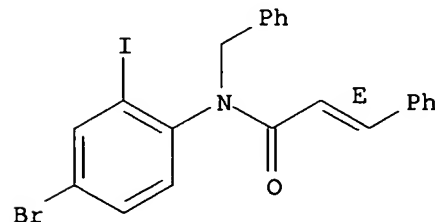
Double bond geometry as shown.



RN 370558-17-1 CAPLUS

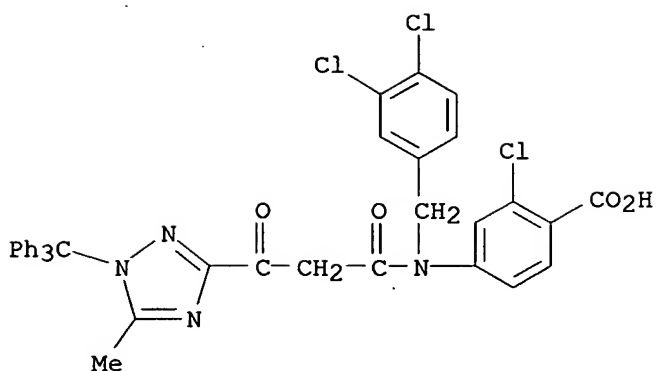
CN 2-Propenamide, N-(4-bromo-2-iodophenyl)-3-phenyl-N-(phenylmethyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 370558-37-5 CAPLUS

CN 2-Propenamide-2-d, N-(2-iodo-4-methylphenyl)-3-phenyl-N-(phenylmethyl)-, (2E)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 37 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:40168 CAPLUS

DOCUMENT NUMBER: 138:89828

TITLE: Preparation of octahydro-2H-pyrido[1,2-a]pyrazine derivatives as H3 receptor antagonists, process for their preparation and pharmaceutical compositions containing them

INVENTOR(S): Goldstein, Solo; Poissonnet, Guillaume; Parmentier, Jean-Gilles; Lestage, Pierre; Lockhart, Brian

PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.

SOURCE: Eur. Pat. Appl., 52 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

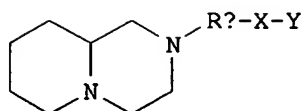
LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

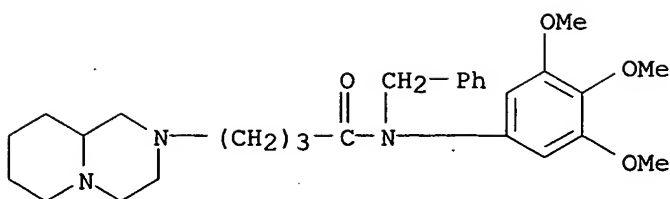
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EP 1275647	A1	20030115	EP 2002-291745	20020711
EP 1275647	B1	20031112		
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FR 2827288	A1	20030117	FR 2001-9260	20010712
FR 2827288	B1	20031031		
JP 2003064081	A2	20030305	JP 2002-201793	20020710
NO 2002003345	A	20030113	NO 2002-3345	20020711
BR 2002002681	A	20030506	BR 2002-2681	20020711
AT 254124	E	20031115	AT 2002-291745	20020711
NZ 520120	A	20040326	NZ 2002-520120	20020711
PT 1275647	T	20040331	PT 2002-291745	20020711
ES 2210219	T3	20040701	ES 2002-2291745	20020711
CN 1397557	A	20030219	CN 2002-124148	20020712
ZA 2002005596	A	20030327	ZA 2002-5596	20020712
US 2003195216	A1	20031016	US 2002-195019	20020712
PRIORITY APPLN. INFO.:			FR 2001-9260	A 20010712
OTHER SOURCE(S):			MARPAT 138:89828	

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I

- AB Octahydro-2H-pyrido[1,2-a]pyrazine derivs. (shown as I; variables defined below; e.g. 4-(3-octahydro-2H-pyrido[1,2-a]pyrazin-2-ylpropoxy)benzonitrile difumarate), methods of preparation, pharmaceutical compns. containing them and their activity as H3 receptor antagonists are disclosed. ≥80 Example preps. of I are included. For example, 2-[4-(3,4,5-trimethoxyphenoxy)butyl]octahydro-2H-pyrido[1,2-a]pyrazine dihydrochloride was prepared starting from 3,4,5-trimethoxyphenol and Et 4-bromobutanoate via intermediates Et 4-(3,4,5-trimethoxyphenoxy)butanoate, 4-(3,4,5-trimethoxyphenoxy)butanoic acid and 1-(octahydro-2H-pyrido[1,2-a]pyrazin-2-yl)-4-(3,4,5-trimethoxyphenoxy)butan-1-one. Doses of 30 mg/kg IP of 2-[4-(1H-benzimidazol-1-yl)butyl]octahydro-2H-pyrido[1,2-a]pyrazine trihydrochloride, and 2-[4-(1H-indazol-1-yl)butyl]octahydro-2H-pyrido[1,2-a]pyrazine dihydrochloride increase the endogenous cerebral concentration of N-methylhistamine by 89% and 124%, resp.; doses of 10 mg/kg IP of 4-(3-octahydro-2H-pyrido[1,2-a]pyrazin-2-ylpropoxy)benzonitrile difumarate and one enantiomer of 4-(3-octahydro-2H-pyrido[1,2-a]pyrazin-2-ylpropoxy)benzonitrile difumarate increase the endogenous cerebral concentration of N-methylhistamine by 252% and 236%, resp. For I: Ra = (C1-C6) linear or branched alkylene chain. X = W1, -C(W1)-W2-, -W2-C(W1)-, -W2-C(W1)W2-, -W2-Ra-, and -CH(OR1)- (W1 = O, S, or -NR2 (R2 = H, (C1-C6) linear or branched alkyl, aryl, (C1-C6) linear or branched arylalkyl, and (C1-C6) linear or branched acyl; W2 = W1; R1 = H and (C1-C6) linear or branched alkyl)) when Y = aryl or heteroaryl. Or X = simple bond, -C(W1)-, -W2-C(W1)-, -W2-Ra-, and -CH(OR1) when Y = fused bicycle (the ring attached to X = unsatd. or partially saturated N heterocycle with 4-7 members containing optionally a 2nd heteroatom = O, N, S, and optionally substituted by ≥1 oxo and (C1-C6) linear or branched alkyl; the 2nd ring = Ph optionally substituted by ≥1 halo, nitro, cyano, hydroxy, (C1-C6) alkoxy, (C1-C6) alkyl, (C1-C6) trihaloalkyl, (C1-C6) acyl, (C1-C6)acyloxy, carboxy, (C1-C6)alkoxycarbonyl, mercapto, (C1-C6)alkylthio, and amino optionally substituted by 1-2 (C1-C6)alkyl, aryl, and (C1-C6)arylalkyl). Conditions treatable using I include cognitive deficit associated with cerebral aging, neurodegenerative maladies, obesity, convulsions, attention deficit hyperactivity disorder, etc.
- IT **484675-90-3P**, N-Benzyl-4-(octahydro-2H-pyrido[1,2-a]pyrazin-2-yl)-N-(3,4,5-trimethoxyphenyl)butyramide  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of octahydro-2H-pyrido[1,2-a]pyrazine derivs. as H3 receptor antagonists, process for their preparation and pharmaceutical compns. containing them)
- RN 484675-90-3 CAPLUS
- CN 2H-Pyrido[1,2-a]pyrazine-2-butanamide, octahydro-N-(phenylmethyl)-N-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



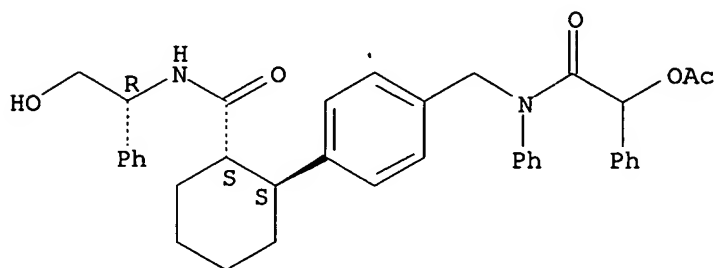
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 38 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:927401 CAPLUS  
 DOCUMENT NUMBER: 138:14016  
 TITLE: Preparation of isoindole and isoquinoline derivatives as inhibitors of Factor xa  
 INVENTOR(S): Zhang, Penglie; Zhu, Bing-Yan; Huang, Wenrong; Scarborough, Robert M.  
 PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA  
 SOURCE: PCT Int. Appl., 72 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096873	A1	20021205	WO 2002-US16784	20020529
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003114448	A1	20030619	US 2002-171804	20020528
PRIORITY APPLN. INFO.:			US 2001-294273P	P 20010531
OTHER SOURCE(S):		MARPAT 138:14016		
GI				

diseases)  
RN 432046-62-3 CAPLUS  
CN Benzeneacetamide,  $\alpha$ -(acetyloxy)-N-[[4-[(1S,2S)-2-[[[(1R)-2-hydroxy-1-phenylethyl]amino]carbonyl]cyclohexyl]phenyl]methyl]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 46 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:173320 CAPLUS  
DOCUMENT NUMBER: 136:363255  
TITLE: GBR Compounds and Mepyramines as Cocaine Abuse  
Therapeutics: Chemometric Studies on Selectivity Using  
Grid Independent Descriptors (GRIND)  
AUTHOR(S): Benedetti, Paolo; Mannhold, Raimund; Cruciani,  
Gabriele; Pastor, Manuel  
CORPORATE SOURCE: Dipartimento di Chimica, Laboratorio di Chemiometria,  
Universita di Perugia, Perugia, I-06123, Italy  
SOURCE: Journal of Medicinal Chemistry (2002), 45(8),  
1577-1584  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

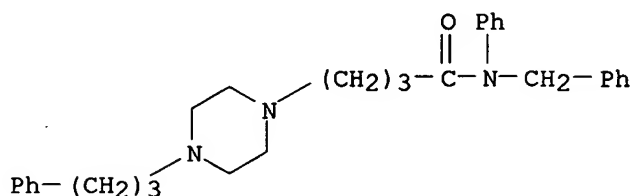
AB Cocaine is one of the most widely abused drugs in the industrial world. Substantial evidence has accumulated that the dopamine transporter (DAT) is a key target for cocaine regarding its reinforcing effects. This work describes the application of chemometric methods to a data set of 54 N1-benzhydryl-oxy-alkyl-N4-phenyl-alk(en)yl-piperazines (GBR compds.) and chemical related mepyramines as putative candidates in cocaine abuse therapy. The aim of the study is to gain insight into the structural requirements that determine the affinity of the data set mols. to the DAT and the serotonin transporter (SERT) as well as their inhibitory potency on dopamine uptake. The compds. in the dataset are described using the recently developed GRID independent descriptors (GRIND), which allow one to obtain fast three-dimensional quant. structure-activity relation models without the need of aligning and superimposing the structures; the results are interpreted in a convenient pharmacophoric-like fashion. In the first part of the work, the selectivity of the database mols. for DAT binding vs. dopamine reuptake inhibition is investigated. In the second part, the selectivity of the compds. for DAT binding vs. SERT binding is studied. In both cases, significant models are obtained, which define the structural features responsible for the resp. selectivity profiles. Moreover, the information has potential interest for the design of new derivs. with improved selectivity.

IT 422575-12-0 422575-16-4 422575-17-5  
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(chemometric studies on GBR compds. and mepyramines as cocaine abuse therapeutics)

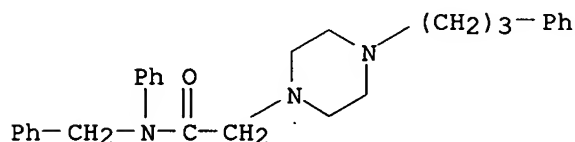
RN 422575-12-0 CAPLUS

CN 1-Piperazinebutanamide, N-phenyl-N-(phenylmethyl)-4-(3-phenylpropyl)-  
(9CI) (CA INDEX NAME)



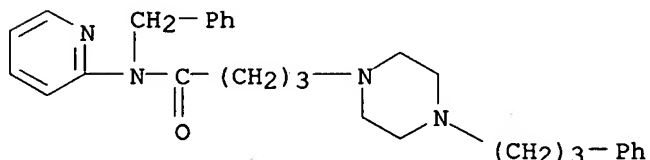
RN 422575-16-4 CAPLUS

CN 1-Piperazineacetamide, N-phenyl-N-(phenylmethyl)-4-(3-phenylpropyl)- (9CI)  
(CA INDEX NAME)



RN 422575-17-5 CAPLUS

CN 1-Piperazinebutanamide, N-(phenylmethyl)-4-(3-phenylpropyl)-N-2-pyridinyl-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 47 OF 174 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:122938 CAPLUS

DOCUMENT NUMBER: 136:183619

TITLE: Preparation of diphenyl ether amides, oxamides, and ureas for treatment of arteriosclerosis and hypercholesterolemia.

INVENTOR(S): Haning, Helmut; Pernerstorfer, Josef; Schmidt, Gunter; Woltering, Michael; Bischoff, Hilmar; Voehringer, Verena; Kretschmer, Axel; Faeste, Christiane

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 169 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

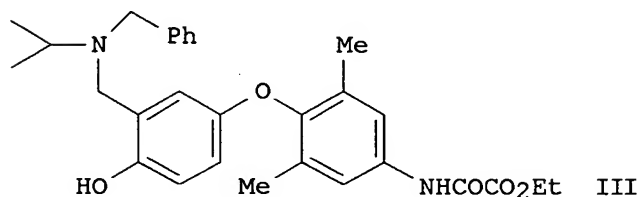
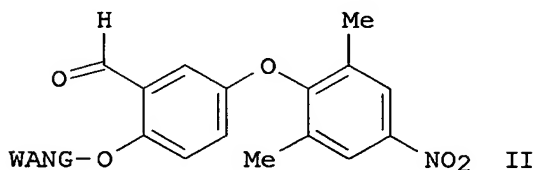
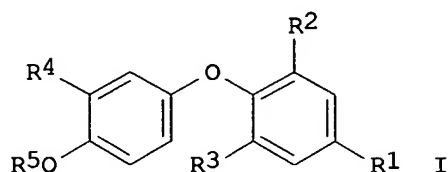
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2002012169      A1      20020214      WO 2001-EP8477      20010723  
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
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HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
DE 10038007      A1      20020214      DE 2000-10038007      20000804  
AU 2001078502      A5      20020218      AU 2001-78502      20010723  
CA 2417880      AA      20030131      CA 2001-2417880      20010723  
EP 1307426      A1      20030507      EP 2001-956554      20010723  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
US 2003027862      A1      20030206      US 2001-918741      20010731  
US 6555580      B2      20030429  
PRIORITY APPLN. INFO.:      DE 2000-10038007      A      20000804  
WO 2001-EP8477      W      20010723  
OTHER SOURCE(S):      MARPAT 136:183619  
GI



AB Title compds. [I; R1 = NO2, amino, acetamido, NHCOCOA, NHCH2COA; A = OH, alkoxy; R2, R3 = halo, alkyl, CF3; R4 = ENR6R7, ENR9COR8, NHCOR10, CONR11R12; E = alkylene; R6, R7 = (substituted) alkyl, aryl, cycloalkyl, heterocyclyl; R6R7N = heterocyclyl; R8 = (substituted) alkyl, cycloalkyl, aryl, biphenyl, alkoxy; R9 = (substituted) alkyl optionally interrupted by O, cycloalkyl, alkenyl, Ph, pyridyl; R8R9 = atoms to form a 4-7 membered heterocyclyl; R10 = (substituted) alkyl, cycloalkyl, aryl, 5-6 membered (aromatic), (benzoannellated) heterocyclyl; R11, R12 = H, (substituted) alkyl, cycloalkyl, 5-7 membered heterocyclyl; R11R12N = 5-7 membered (benzoannellated) (substituted) (aromatic) heterocyclyl], were prepared Thus, resin-bound substrate (II) was converted to title compound (III) in several steps using isopropylamine, benzyl chloride, and ethoxalyl chloride.